UNIVERSITY OF MARIBOR
FACULTY OF CHEMISTRY AND CHEMICAL ENGINEERING

PhD – Doctoral Dissertation

SYNTHESIS OF SUSTAINABLE BIOPROCESSES USING COMPUTER-AIDED PROCESS ENGINEERING

Maribor, March 2013

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Doktorska disertacija

SINTEZA TRAJNOSTNIH BIOPROCESOV Z UPORABO RAČUNALNIŠKO PODPRTE PROCESNE TEHNIKE

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Science is a way of thinking much more than it is a body of knowledge
Carl Sagan

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SKLEP O IMENOVANJU KOMISIJE ZA ZAGOVOR DOKTORSKE DISERTACIJE

z naslovom
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podprte procesne tehnike

ki jo je predložila Lidija Čuček, univ. dipl. inž. kem. tehnol.

V komisijo imenujem naslednje člane:

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Če imenovani član komisije zavrne sodelovanje v komisiji za zagovor doktorske disertacije, mora o tem v roku 5 delovnih dni po prejemu tega sklepa pisno obvestiti dekana članice.

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ABSTRACT

This doctoral dissertation, which consists of four substantive wholes, presents several syntheses of sustainable bioprocesses using computer-aided process engineering. The first part presents the synthesis of different integrated processes of ethanol production from the entire corn plant. The synthesis of different processes is further extended in the second part into the simplified synthesis and the more comprehensive synthesis of bioproducts within the whole production supply chain network. Synthesis is based on the generic optimisation model of biomass production and supply chain networks.

In the third part, three methods are presented for sustainable development assessment, suitable for multi-criteria optimisation: the methods of sustainability indexes, footprints, and combined criteria, such as eco- and total profit. These methods are further upgraded according to their indirect unburdening effects, in order to measure any unburdening of the environment, associated with the usage and replacement of environmentally-harmful products. These methods include direct, indirect, and total impacts on the environment.

The final part presents the methodology for reducing of a large number of criteria within multi-objective optimisation to a smaller number of representative criteria. This method is presented on the case of environmental footprints.

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Keywords: Biomass energy generation, Supply chain networks, Synthesis of sustainable bioprocesses, Life Cycle Analysis, Sustainability assessment, Multi-objective optimisation, Dimensionality reduction, Representative Objectives Method

KLJUČNA DOKUMENTACIJSKA INFORMACIJA

ŠD	Dd
DK	UDK: 66.011:66.098:502.131.1(043.3)
KS	matematično programiranje / sinteza / optimiranje / bioenergija / dobavna veriga / trajnostni razvoj / zmanjšanje dimenzionalnosti
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AV	ČUČEK, Lidija
SA	KRAVANJA, Zdravko (mentor), KLEMEŠ, Jiří Jaromír (somentor)
KZ	SI-2000 Maribor, Smetanova 17
ZA	Univerza v Mariboru, Fakulteta za kemijo in kemijsko tehnologijo
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IN	SINTEZA TRAJNOSTNIH BIOPROCESOV Z UPORABO RAČUNALNIŠKO PODPRTE PROCESNE TEHNIKE
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IJ	en
JI	en/sl

POVZETEK

V doktorski disertaciji, ki zajema 4 sklope, predstavljamo sintezo več trajnostnih bioprocesov z uporabo računalniško podprte procesne tehnike. V prvem delu je predstavljena sinteza različnih integriranih procesov proizvodnje etanola iz celotne koruzne rastline. Sinteza različnih procesov je nato v drugem delu razširjena na poenostavljeno in celovitejšo sintezo bioproduktov v celotni proizvodni mreži. Le-ta temelji na splošnem optimizacijskem modelu omrežja za proizvodnjo in dobavo biomase in biogoriv.

V tretjem delu so predstavljene tri metode ocenjevanja trajnostnega razvoja, primerne za večkriterijsko optimiranje: metoda trajnostnih indeksov, metoda odtisov in kombinirani kriteriji, kot sta metoda eko- in celotnega dobička. Metode so nato nadgrajene tako, da upoštevajo tudi posredne razbremenilne okoljske vplive, povezane z rabo in zamenjavo okolju škodljivih produktov. Metode tako vključujejo neposredne, posredne in celotne vplive na okolje.

V zadnjem delu je predstavljena metodologija za zmanjšanje večjega števila kriterijev pri večkriterijskem optimiranju na manjše število reprezentativnih kriterijev. Metoda je predstavljena na primeru okoljskih odtisov.

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Ključne besede: Proizvodnja energije iz biomase, Omrežja dobavnih verig, Sinteza trajnostnih bioprocesov, Analiza življenjskega kroga, Ocenjevanje trajnostnega razvoja, Večkriterijsko optimiranje, Zmanjšanje dimenzionalnosti, Metoda reprezentativnih kriterijev

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SYMBOLS

Superscripts

add	Additional resource
buy	Purchased resource
C	Constrained remaining footprints
conv	Conversion
cost	Cost of the raw material
d	Direct
fix	Fixed part of the annualised investment
ind	Indirect
inv	Investment cost
L1	Harvesting and supply layer
L2	Collection, pre-processing and storage layer
L3	Main processing layer
L4	Use layer
LO	Lower bound
net	Net flowrate
op	Operating cost
pretreat	Pretreatment
price	Price of the product
r	Relative
R	Relaxed remaining footprints
road	Road conditions
spod	Storage, preprocessing, operating and depreciation cost
stor	Storage
t	Total
T	Technology
tr	Transport
s	Specific
sub	Substituted product
UP	Upper bound
var	Cost coefficient of the annualised investment
0	Reference or base-case

Sets

FP	Set of footprints
FR	Set of representative footprints
FS	Set of similar footprints
FU	Set of unrepresentative remaining footprints
I	Set of supply zones
J	Set of demand locations
K	Set of iterations
M	Set of collection, storage and pre-processing facilities
N	Set of process plants
NI	Set of intervals
O	Set of objectives
P	Set of products
PS	Set of substituted products
P_{B}	Set of those products that only burden the environment in relation to processing, disposal and transportation
P_{UNB}	Set of those products that burden and unburden the environment when used
R_{B}	Set of those raw materials that only burden the environment if processed
R_{UNB}	Set of those raw materials that burden and unburden the environment when used
S	Set of groups (subsets) of similar footprints
T	Set of technology options
TP	Set of time periods
V	Set of variables

Subsets

KP	Set of key products ($KP \subseteq (PM \cup PP)$)
$PADD$	Set of additional resources needed for conversion besides main resources $(PADD \subseteq P = PBUY \cup POUTPIN)$
$PBUY$	Set of purchased raw materials $(PBUY \subseteq P)$
PD	Set of directly used products $(PD \subseteq P)$
PI	Set of intermediate products $(PI \subseteq P)$
$PICON$	Set of year-round resources $(PICON \subseteq PI)$
$PIPM$	Set of pairs of resource and pre-treated product (if a pre-treated product is from a given resource) with elements $(pi, pm) \in PIPM$
$PIPP$	Set of intermediate and produced product (if a produced product is from a given intermediate product) with elements $(pi, pp) \in PIPP$
$PISE$	Set of seasonal biomass resources $(PISE \subseteq PI)$
PIT	Set of pairs of intermediate product, and the applicable process technology for it with elements $(pi, t) \in PIT$
PM	Set of stored and pre-treated products (intermediate products) from storage and pre-processing facilities $(PM \subseteq P)$
$PMPP$	Set of intermediate and produced product (if a produced product is from a given intermediate product) with elements $(pm, pp) \in PMPP$
PMT	Set of pairs of product pm, and the applicable process technology for it with elements $(pm, t) \in PMT$
$POUTPIN$	Set of recycled produced products from technology t to technology tt $(POUTPIN \subseteq P)$
PP	Set of produced products from plants $(PP \subseteq P)$
PPT	Set of pairs of produced product pp, and its applicable process technology with elements $(pp, t) \in PPT$
PSP	Set of pairs of substituted product and produced product (if a produced product substitutes conventional product) with elements $(ps, pp) \in PSP$
T_2	Set of technology options at pre-processing facilities $(T_2 \subseteq T)$
T_3	Set of technology options at processing plants $(T_3 \subseteq T)$
TKP	Set of pairs of technology and produced key product (if a key product is produced from a given technology) with elements $(t, kp) \in TKP$
$TTPADD$	Set of pairs of technology and additional resource needed (if an additional resource is needed for a given technology) with elements $(padd, tt) \in TTPADD$

Subsets

TTTNM	Set of quintuples of locations *n* and *m*, technologies *t* at L3 and *tt* at L2, and recycled produced product *poutpin* (if product is recycled from technology *t* at L3 to technology *tt* at L2) with elements $(n, m, t, tt, poutpin) \in TTTNM$
TTTP	Set of quintuples of locations *n* and *nn*, technologies *t* at *n*, and *tt* at *nn*, and recycled produced product *poutpin* (if product is recycled from technology *t* at *n* to technology *tt* at *nn*) with elements $(n, nn, t, tt, poutpin) \in TTTP$.
UTILITY	Set of process utilities $(UTILITY \subseteq P)$

Indexes

f	Index for footprints
fr	Index for representative footprints
fs	Index for similar footprints
fu	Index for unrepresentative remaining footprints
i	Index for supply zones
j	Index for demand locations
k	Index for iterations
kp	Index for key products
m	Index for collection, storage and pre-processing facilities
n	Index for process plants
ni	Index for interval numbers
o	Index for objectives
p	Index for products
$padd$	Index for additional resources needed for conversion besides main resources
$pbuy$	Index for purchased raw materials
pd	Index for directly used products
pi	Index for intermediate products
$picon$	Index for year-round resources
$pise$	Index for seasonal biomass resources
pm	Index for pre-treated and stored resource
$poutpin$	Index for recycled produced products from technology t to technology tt
pp	Index for produced products
ps	Index for substituted products
s	Index for similar footprints
t	Index for technology options
tp	Index for time period
$utility$	Index for process utility
v	Index for variables

Scalars

A	Supply chain network's total area, km^2
$q^{m,\mathrm{L2}}$	Total mass-flow at collection centre m, t/y
$\|K\|$	Cardinality of a set K (the number of iterations k)
N_i	The size of set I
N_j	The size of set J
N_k	Number of obtained feasible solutions from K iterations
N_m	The size of set M
N_n	The size of set N
N_s	Number of subsets (groups) of similar footprints (and embedded loop statements)
$\|NI\|$	Cardinality of a set NI (the number of intervals ni)
ny	Number of project lifetime y
sf	Scale factor
$\|TP\|$	Cardinality of a set TP (the number of time periods tp)
w	Small weight in objective function to simultaneously minimise footprint values
$w_{\mathrm{H_2O}}$	Mass fraction of water, -
ε	ε-constraint

Parameters

$a_{f,v}$	Matrix coefficient (Specific environmental footprint)
A_i^{UP}	Total available area of zone *i*, km^2
$AD_{f,ff,k}$	Arithmetic mean of average absolute normalised deviation between pairs of footprints *f* and *ff* for selected optimal point x_k
$AD^{\mathrm{m}}_{f,ff}$	Mean value of the arithmetic mean of average absolute normalised deviation between pairs of footprints *f* and *ff*
c_p^{cost}	Cost for each raw material *pi*, monetary unit (m.u.)/t
$c_{p,t}^{\mathrm{op,T}}$	Operating cost for product *p* and technology *t*, m.u./t
c_p^{s}	Eco-cost or eco-benefit coefficient for each raw material and product *p*, m.u./t or m.u./MJ
$c_p^{\mathrm{s,tr}}$	Eco-cost or eco-benefit coefficient for each raw material and product *p* for transportation, m.u./(t·km) or m.u./(m^3·km)
$c_p^{\mathrm{tr,fix,L}a\mathrm{,L}b}$	Fixed transportation cost coefficient of product from layer *a* to the layer *b*, m.u./t
$c_p^{\mathrm{tr,var,L}a\mathrm{,L}b}$	Variable transportation cost coefficient of product from layer *a* to the layer *b*, m.u./(t·km)
$c_{p,tp}^{\mathrm{price}}$	Price of the product in time period *tp*, m.u./t or m.u./MWh or m.u./MJ
$c_{pm}^{\mathrm{pretreat}}$	Unit pretreatment cost for product *pm*, m.u./t
c_p^{stor}	Storage cost for product *p*, m.u./t
$D_{f,ff,k}$	Average absolute normalised deviation between pair of footprints *f* and *ff* for selected optimal point x_k
$D^{\mathrm{m}}_{f,ff}$	Mean value of average absolute normalised deviation between pair of footprints *f* and *ff*
D_p	Distance between the locations for transporting product *p*, km
$D_{x,y}^{\mathrm{L}a\mathrm{,Lb}}$	Distance between object *x* in layer *a* and object *y* in layer *b*, km
Dem_p	Regional annual demand for product *p*, t/y, GJ/y, MWh/y
$Det_{p,tp}$	Product’s deterioration percentage per time period *tp*, %/(y·|*TP*|)
$ei_{f,pi}^{\mathrm{L}a}$	Specific environmental footprint *f* of intermediate product *pi* at layer *a*, $a=\{1,2\}$, kg/(t·km^2) or GJ/(t·km^2) or 1/t
$ei_{f,pi,t}^{\mathrm{L3}}$	Specific environmental footprint *f* of intermediate product *pi* and the selected technology *t* at processing layer, kg/(t·km^2) or MJ/(t·km^2) or 1/t
$ei_{f,p}^{\mathrm{L4}}$	Specific environmental footprint *f* of product *p* at use layer, kg/(t·km^2) or GJ/(t·km^2) or 1/t

Parameters

$ei^{\mathrm{sub}}_{f,ps}$	Specific environmental footprint *f* of substituted product *ps*, (t or GJ)/(MWh or GJ or t)
$ei^{\mathrm{tr},\mathrm{L}a,\mathrm{L}b}_{f,p}$	Transport environmental footprint *f* from layer *a* to the layer *b*, kg/(t·km^3) or GJ/(t·km^3) or 1/(t·km)
$F^0_f(x)$	Footprint obtained at maximum profit solution, where footprints are relaxed, t/(km^2·y) or GJ/(km^2·y) or km^2/(km^2·y)
$f^{S/P_{\mathrm{UNB}}}_p$	Substitution factor between the conventional product *S* and biomass product P_{UNB}
$f^{\mathrm{conv},\mathrm{L2}}_{pi}$	Conversion factor of intermediate product *pi* by pre-processing
$f^{\mathrm{conv},\mathrm{T},\mathrm{L2}}_{pi,pm,t}$	Conversion factor of resource *pi* to pre-treated product *pm* by pre-processing
$f^{\mathrm{conv},\mathrm{T},\mathrm{L3}}_{pm,pp,t}$	Conversion factor of pre-treated product *pm* to produced product *pp* by processing
$f^{\mathrm{sub}}_{ps,pp}$	Substitution factor between the conventional energy *ps* and biomass energy *pp*
$f^{\mathrm{conv},\mathrm{add},\mathrm{T}}_{t,padd,kp}$	Conversion factor of additional resource *padd* to produced key product *kp* by technology *t*
$f^{\mathrm{road},\mathrm{L}a,\mathrm{L}b}_{x,y}$	Road condition factor between object *x* in layer *a* and object *y* in layer *b*
$GO_{f,ff,k}$	Geometric mean of overlap of pairs of footprints *f* and *ff* in process variables for selected optimal point x_k
$GO^{\mathrm{m}}_{f,ff}$	Mean value of the geometric mean of overlap of pairs of footprints *f* and *ff* in process variables
$GR_{f,ff,k}$	Geometric mean of normalised ratio between pairs of footprints *f* and *ff* for selected optimal point x_k
$GR^{\mathrm{m}}_{f,ff}$	Mean value of the geometric mean of normalised ratio between pairs of footprints *f* and *ff*
$HY_{pi,tp}$	Yield for product *pi* in time period *tp*, t/(km^2·(y·|*TP*|))
$I^{\mathrm{s}}_{o,p}$	Specific sustainability indicator *o* for each raw material and product *p*, kg/t or ha/t, …
$I^{\mathrm{s,tr}}_{o,p}$	Specific sustainability indicator *o* for each raw material and product *p* for transportation, kg/(t·km), kg/(m^3·km), …
$I^{\mathrm{T,L2}}_{m,kp,t,ni}$	Capital cost for technology *t* in regards to key product *kp* at L2 in interval *ni*, m.u.
$I^{\mathrm{T,L3}}_{n,kp,t,ni}$	Capital cost for technology *t* in regards to key product *kp* at L3 in interval *ni*, m.u.
I^{T}_t	Capital cost for the technology *t*, m.u.
$I^{\mathrm{T},0}_t$	Capital cost for the technology *t* by its reference capacity, m.u.
l_p	Inverse of the load factor for each raw material and product *p*

Parameters

L_p	Harvesting loss, %
L_p^{tr}	Product's loss percentage with the distance, %
$m_{m,kp,t,ni}^{\mathrm{T,L2}}$	The slope of the line for technology *t* in regards to key product *kp* at L2 within interval *ni*
$m_{n,kp,t,ni}^{\mathrm{T,L3}}$	The slope of the line for technology *t* in regards to key product *kp* at L3 within interval *ni*
o_k^{C}	Objective by constrained remaining footprints at iteration *K*
o_k^{R}	Objective by relaxed remaining footprints at iteration *K*
$O_{f,ff,k}$	Overlap of pairs of footprints *f* and *ff* in process variables for selected optimal point x_k
$O_{f,ff}^{\mathrm{m}}$	Mean value of the overlap of pairs of footprints *f* and *ff* in process variables
$q_{m,kp,t,ni}^{m,\mathrm{T,L2}}$	Capacity of technology *t* in regards to key product *kp* al L2 in interval *ni*, t/y
$q_{n,kp,t,ni}^{m,\mathrm{T,L3}}$	Capacity of technology *t* in regards to key product *kp* al L3 in interval *ni*, t/y
$q_t^{m,\mathrm{T}}$	Limited capacity of technology *t*, t/y
$q_t^{m,\mathrm{T},0}$	Reference capacity of each process technology *t*, t/y
$q_{t,tp}^{m,\mathrm{T}}$	Limited capacity of technology *t* per time period *tp*, t/(y·|*TP*|)
$R_{f,ff,k}$	Normalised ratio between pairs of footprints *f* and *ff* for selected optimal point x_k
$R_{f,ff}^{\mathrm{m}}$	Mean value of the normalised ratio between pairs of footprints *f* and *ff*
w_o	Weighting factor for objective *o*
x_i	Fraction of area intended for energy in zone *i*
$\delta_{o,k}^{\mathrm{C}}$	Delta percentage for each feasible objective o when the remaining footprints are constrained, at each iteration k
$\delta_{o,k}^{\mathrm{R}}$	Delta percentage for each feasible objective o when the remaining footprints are relaxed, at each iteration k
ε_k	ε-constraint depending on iteration *k*
$\varepsilon_{s,k}$	ε-constraint for each representative footprint depending on iteration *k*
μ_o^{C}	The means of errors for constrained solutions for each feasible objective o
μ_o^{R}	The mean of errors for relaxed solutions for each feasible objective o
σ_o^{C}	Standard deviation for constrained solutions for each feasible objective o
σ_o^{R}	Standard deviation for relaxed solutions for each feasible objective o

Variables

$A_{i,pi}$	Area available for growing biomass resources *pi* at zone *i*, km^2
$A_{i,pi,tp}$	Area available for growing raw materials *pi* at zone *i* in each time period *tp*, km^2
c^{Eco}	Annual eco-cost, m.u./y
c^{spod}	Sum of storage, pre-processing and operating cost, and annual depreciation expense, m.u./y
c^{stor}	Storage cost, m.u./y
c^{tr}	Total transportation cost, m.u./y
$c_p^{\mathrm{tr,L}a\mathrm{,L}b}$	Transportation cost of product from layer *a* to the layer *b*, m.u./y
$c_{pm,t}^{\mathrm{pretreat,T}}$	Pre-treatment cost of production *pm*, m.u./y
$c_t^{\mathrm{op,T}}$	Operating cost for the technology *t*, m.u./(y·|*TP*|)
$f(x)$	Continuous function involved in objective function
F_f	Total environmental footprint type *f*, t/(km^2·y) or GJ/(km^2·y) or km^2/(km^2·y)
F_f^{ind}	Indirect environmental footprint type *f*, t/(km^2·y) or GJ/(km^2·y) or km^2/(km^2·y)
$F_f^{\mathrm{L}a}$	Direct environmental footprint type *f* at layer *a*, t/(km^2·y) or GJ/(km^2·y) or km^2/(km^2·y)
F_f^{tr}	Direct environmental footprint type *f* related to transportation, t/(km^2·y) or GJ/(km^2·y) or km^2/(km^2·y)
$F_{f,k}(x)$	Environmental footprint obtained by optimisation depending on iteration *k*, t/(km^2·y) or GJ/(km^2·y) or km^2/(km^2·y)
$F_{f,k}^{r}(x)$	Relative footprint obtained by optimisation depending on iteration *k*, t/(km^2·y) or GJ/(km^2·y) or km^2/(km^2·y)
$g(x,y)$	Continuous inequality constraints function
$h(x,y)$	Continuous equality constraints function
$I_{m,t}^{\mathrm{T,L2}}$	Capital cost for technology *t* at L2, m.u.
$I_{n,t}^{\mathrm{T,L3}}$	Capital cost for technology *t* at L3, m.u.
I_o	Sustainability indicator
I_o^{d}	Direct sustainability indicator
I_o^{ind}	Indirect sustainability indicator
I_o^{t}	Total sustainability indicator
$m_{m,pm,tp}^{\mathrm{L2}}$	The quantity of stored intermediate product *pm* at L2 at time period *tp*, t
$m_{m,pm}^{\mathrm{L2,UP}}$	Maximal storage capacity of intermediate product *pm* at L2, t
$m_{n,t,pp,tp}^{\mathrm{L3}}$	The quantity of stored produced product *pp* at L3 at time period *tp*, t

Variables

$m_{n,t,pp}^{\mathrm{L3,UP}}$	Maximal storage capacity of produced product *pp* at L3, t
P, P^{Econ}	Economic profit before tax, m.u./y
P^{Eco}	Annual eco-profit, m.u./y
P^{N}	Annual net profit, m.u./y
P^{T}	Annual total profit, m.u./y
P_k	Profit obtained by iteration *k*, m.u./y
R^{Eco}	Annual eco-benefit or eco-revenue, m.u./y
$q_{i,pi}^{m,\mathrm{L1}}$	Production rate of resource *pi* at supply zone *i*, t/y
$q_{i,pi,tp}^{m,\mathrm{L1}}$	Production rate of resource *pi* at supply zone *i* and at time period *tp*, t/(y·|*TP*|)
$q_{m,pi,pm,t}^{m,\mathrm{T,L2}}$	Flowrate of intermediate material *pm* from raw material *pi* with the selected technology *t* at the pre-processing and storage facility *m*, t/y
$q_{m,pi,pm,t,tp}^{m,\mathrm{T,L2}}$	Flowrate of pre-treated product *pm* from raw material *pi* with the selected technology *t* at the pre-processing facility *m*, at time period *tp*, t/(y·|*TP*|)
$q_{m,pi,pm,t}^{m,\mathrm{T,L2,UP}}$	Maximal flowrate of pre-treated product *pm* from raw material *pi* with the selected technology *t* at the pre-processing facility *m*, t/y
$q_{m,pi,t,tp}^{m,\mathrm{T,L2}}$	Flowrate of biomass type *pi* to the selected technology *t* at the pre-processing and storage facility *m* at time period *tp*, t/(y·|*TP*|)
$q_{m,t,pbuy,tp}^{m,\mathrm{buy,T,L2}}$	Flowrate of purchased raw material *pbuy* to the selected technology *t* at L2 at time period *tp*, t/(y·|*TP*|)
$q_{n,m,t,tt,poutpin,tp}^{m,\mathrm{T,L3,L2}}$	Flowrate of recycled produced product *poutpin* from technology *t* at L3 to the selected technology *tt* at L2 at time period *tp*, t/(y·|*TP*|)
$q_{n,m,t,tt,poutpin,tp}^{m,\mathrm{net,T,L3,L2}}$	Net flowrate of recycled produced product *poutpin* from technology *t* at L3 to the selected technology *tt* at L2 at time period *tp*, t/(y·|*TP*|)
$q_{n,nn,t,tt,poutpin,tp}^{m,\mathrm{T,L3,L3}}$	Flowrate of recycled produced product *poutpin* from technology *t* at L3 to the selected technology *tt* at L3 at time period *tp*, t/(y·|*TP*|)
$q_{n,nn,t,tt,poutpin,tp}^{m,\mathrm{net,T,L3,L3}}$	Net flowrate of recycled produced product *poutpin* from technology *t* at L3 to the selected technology *tt* at L3 at time period *tp*, t/(y·|*TP*|)
$q_{n,pi,pp,t}^{m,\mathrm{T,L3}}$	Flowrate of produced product *pp* from intermediate product *pi* with the selected technology *t* at the process plant *n*, t/y
$q_{n,pi,t}^{m,\mathrm{T,L3}}$	Flowrate of intermediate product *pi* to the selected technology *t* at the process plant *n*, t/y
$q_{n,pm,pp,t}^{m,\mathrm{T,L3}}$	Flowrate of produced product *pp* from pre-treated product *pm* with the selected technology *t* at the process plant *n*, t/y
$q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}}$	Flowrate of produced product *pp* from pre-treated product *pm* with the selected technology *t* at the process plant *n* at time period *tp*, t/(y·|*TP*|)

Variables

$q^{m,\mathrm{T,L3,UP}}_{n,pm,pp,t}$	Maximal flowrate of produced product *pp* from pre-treated product *pm* with the selected technology *t* at the process plant *n*, t/y
$q^{m,\mathrm{T,L3}}_{n,pm,t,tp}$	Flowrate of intermediate product *pm* to the selected technology *t* at the process plant *n*, at time period *tp*, t/(y·|*TP*|)
$q^{m,\mathrm{buy,T,L3}}_{n,t,pbuy,tp}$	Flowrate of purchased raw material *pbuy* to the selected technology *t* at L3 at time period *tp*, t/(y/|*TP*|)
$q^{m,\mathrm{T,L3,L4}}_{n,t,j,pp,tp}$	Flowrate of produced product *pp* from technology *t* at L3 (plant *n*) to demand location *j* at L4 at time period *tp*, t/(y·|*TP*|)
$q^{m,\mathrm{net,T,L3,L4}}_{n,t,j,pp,tp}$	Net flowrate of produced product *pp* from technology *t* at L3 (plant *n*) to demand location *j* at L4 at time period *tp*, t/(y·|*TP*|)
q^{m}_{p}	Flowrate of raw material or product *p*, t/y, GJ/y, …
$q^{m,\mathrm{L}a,\mathrm{L}b}_{x,y,p}$	Flowrate of product *p* from object *x* in layer *a* to object *y* in layer *b*, t/y
$q^{m,\mathrm{L}a,\mathrm{L}b}_{x,y,p,tp}$	Flowrate of product *p* in time period *tp* from object *x* in layer *a* to object *y* in layer *b*, t/(y·|*TP*|)
W_{NP}	Net present value, m.u.
x	Vector of continuous variables
x_k	Pareto optimal solution
$x_{v,k}$	Optimal values of process variables at iteration *k*
$\Delta q^{m,\mathrm{T,L2}}_{m,kp,t,ni}$	Difference in capacity of technology *t* in regards to key product *kp* al L2 (the distance along the x-axis) within interval *ni*, t/y
$\Delta q^{m,\mathrm{T,L3}}_{n,kp,t,ni}$	Difference in capacity of technology *t* in regards to key product *kp* al L3 (the distance along the x-axis) within interval *ni*, t/y

Binary variables

y	Vector of binary variables
y_{m}^{L2}	Binary variable for operating of collection and intermediate process centre *m*
$y_{m,t}^{\mathrm{T,L2}}$	Binary variable for operating of technology *t* at storage and pre-treatment facility *m*
$y_{m,t}^{\mathrm{T,L2}}$	Binary variable for operating of technology *t* at storage and pre-treatment facility *m*
$y_{m,t,ni}^{\mathrm{T,L2}}$	Binary variable for existence of technology *t* at storage and pre-treatment facility *m* in interval *ni*
$y_{m,t,tp}^{\mathrm{T,L2}}$	Binary variable for operating of technology *t* at storage and pre-treatment facility *m* in time period *tp*
$y_{n,j,pp}^{\mathrm{L3,L4}}$	Binary variable for selection or rejection of the flow from L3 to L4
$y_{n,m,poutpin}^{\mathrm{L3,L2}}$	Binary variable for selection or rejection of the recycle from L3 to L2
$y_{n,nn,poutpin}^{\mathrm{L3,L3}}$	Binary variable for selection or rejection of the recycle from L3 to L3
$y_{n,t}^{\mathrm{T,L3}}$	Binary variable for operating of technology *t* at process plant *n*
$y_{n,t,ni}^{\mathrm{T,L3}}$	Binary variable for existence of technology *t* at process plant *n* in interval *ni*
$y_{n,t,tp}^{\mathrm{T,L3}}$	Binary variable for operating of technology *t* at process plant *n* in time period *tp*

ABBREVIATIONS

AD	Anaerobic digestion
AFEX	Ammonia fibre explosion
AIMMS	Advanced Interactive Multidimensional Modelling System
AML	Algebraic modelling language
AMPL	A Mathematical Programming Language
BAT	Best available techniques
BPLB	Biochemical process for lignocellulosic biomass
C	Cold stream
CF	Carbon footprint
CHP	Combined heat and power
CTEP	Clean Technologies and Environmental Policy
D	Dimensional
DDGS	Distillers dried grains with solubles
DGP	The dry-grind process
EC	European Commission
EISA	Energy Independence and Security Act
EF	Energy footprint
EU	European Union
FEF	Food-to-energy footprint
FT	Fischer-Tropsch
FTDP	Fischer-Tropsch diesel and green gasoline production
GAMS	General Algebraic Modelling System
GCS	Gasification and further catalytic synthesis
GHG	Greenhouse gas emissions
GSF	Gasification and further syngas fermentation
H	Hot stream
HBC	Hydrocarbons
HCV	Higher calorific value
HI	Heat integration
H2P	Hydrogen production
IP	Integer program
ISO	International Organisation for Standardisation
IW	Industrial wastewater
LCA	Life Cycle Assessment, also Life Cycle Analysis
LCCA	Life Cycle Cost Analysis
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LF	Agricultural land footprint
LP	Linear program
m.u.	Monetary unit

M/D	Modelling and decomposition strategy
MEA	Monoethanolamines
MILP	Mixed-integer linear program
MINLP	Mixed-integer non-linear program
MIPSYN	Mixed-Integer Process SYNthesizer
MOO	Multi-objective optimisation
MP	Mathematical programming
MSW	Municipal solid waste
NF	Nitrogen footprint
NLP	Non-linear program
NPV	Net present value
OA/ER	Outer approximation and equality-relaxation algorithm
OECD	Organisation for Economic Co-Operation and Development
PCA	Principal Component Analysis
POST	Parliamentary Office of Science and Technology
PSA	Pressure swing adsorption
RDSI	Relative direct sustainability index
RES	Renewable energy sources
RFA	Renewable Fuels Association
RFS	Renewable Fuel Standard
RISI	Relative indirect sustainability index
RNPV	Relative net present value
ROM	Representative Objectives Method
RPS	Renewable Portfolio Standard
RSI	Relative sustainability index
RTSI	Relative total sustainability index
SD	Sustainable development
SEPI	Sustainable Environmental Performance Indicator
SI	Social indicator
SLCA	Social Life Cycle Assessment
SOO	Single-objective optimisation
SPI	Sustainable Process Index
TS	Total Site
UK	United Kingdom
US	The United States of America
WAR	Waste Reduction Algorithm
WCED	World Commission on Environment and Sustainable Development
WF	Water footprint
WGSR	Water gas shift reactor
WPF	Water pollution footprint
WS	Mass flow-rate of water stream

LIST OF PUBLICATIONS

Doctoral dissertation is mainly based on the following seven papers.

1. Čuček L., Lam H. L., Klemeš J. J., Varbanov P. S., Kravanja Z., 2010, Synthesis of regional networks for the supply of energy and bioproducts, Clean Technologies and Environmental Policy (CTEP), 12(6), 635-645 (IF = 1.753 in 2011) (32 citations on March 9, 2013), the second most cited paper published in CTEP in last years

2. Čuček L., Martín M., Grossmann I. E., Kravanja Z., 2011, Energy, water and process technologies integration for the simultaneous production of ethanol and food from the entire corn plant, Computers and Chemical Engineering, 35(8), 1547-1557 (IF = 2.320 in 2011) (16 citations on March 9, 2013)

3. Čuček L., Varbanov P. S., Klemeš J. J., Kravanja Z., 2012, Total footprints-based multi-criteria optimisation of regional biomass energy supply chains, Energy, 44(1), 135-145 (IF = 3.487 in 2011) (11 citations on March 9, 2013)

4. Čuček L., Drobež R., Pahor B., Kravanja Z., 2012, Sustainable synthesis of biogas processes using a novel concept of eco-profit, Computers and Chemical Engineering, 42, 87-100 (IF = 2.320 in 2011) (6 citations on March 9, 2013)

5. Kravanja Z., Čuček L., 2013, Multi-objective optimisation for generating sustainable solutions considering total effects on the environment, Applied Energy, 101, 67-80 (IF = 5.106 in 2011) (5 citations on March 9, 2013)

6. Čuček L., Klemeš J. J., Varbanov P. S., Kravanja Z., 2013, Dealing with high-dimensionality of criteria in multiobjective optimization of biomass energy supply network, Industrial and Engineering Chemistry Research, doi: 10.1021/ie302599c (IF = 2.237 in 2011)

7. Čuček L., Martín M., Grossmann I. E., Kravanja Z., 2013, Multi-period synthesis of optimally-integrated biomass and bioenergy supply network, Computers and Chemical Engineering (IF = 2.320 in 2011)

There are also author’s other papers which may be referred in the thesis:

8. Čuček L., Kravanja Z., 2010, Sustainable LCA-based MINLP synthesis of bioethanol processes, Computer Aided Chemical Engineering, 28, 1889-1894 (4 citations on March 9, 2013)

9. Čuček L., Lam H. L., Klemeš J. J., Varbanov P. S., Kravanja Z., 2010, Synthesis of networks for the production and supply of renewable energy from biomass, Chemical Engineering Transactions, 21, 1189-1194 (5 citations on March 9, 2013)

10. Čuček L., Martín M., Grossmann I. E., Kravanja Z., 2011, Energy, water and process technologies integration for the simultaneous production of ethanol and food from the entire corn plant, Computer Aided Chemical Engineering, 29, 2004-2008

11. Čuček L., Drobež R., Pahor B., Kravanja Z., 2011, Sustainable LCA-based MIP synthesis of biogas processes, Computer Aided Chemical Engineering, 29, 1999-2003 (1 citation on March 9, 2013)

12. Čuček L., Klemeš J. J., Kravanja Z., 2012, Accessing direct and indirect effects within a LCA based multiobjective synthesis of bioproducts supply chains, Computer Aided Chemical Engineering, 31, 1065-1069

13. Čuček L., Klemeš J. J., Varbanov P. S., Kravanja Z., 2012, Correlations among footprints within biomass energy supply chains, Computer Aided Chemical Engineering, 31, 1397-1401 (1 citation on March 9, 2013)

14. Čuček L., Klemeš J. J., Varbanov P. S., Kravanja Z., 2012, Reducing the dimensionality of criteria in multi-objective optimisation of biomass energy supply chains, Chemical Engineering Transactions, 29, 1231-1236

15. Čuček L., Martín M., Grossmann I. E., Kravanja Z., 2013, Multi-period synthesis of a biorefinery's supply networks, Computer Aided Chemical Engineering, accepted for publication

16. Čuček L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2013, Dimensionality Reduction Approach for Multi-Objective Optimisation Extended to Total Footprints, Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA), Kuala Lumpur, Malaysia, accepted for publication

1 INTRODUCTION

The increasing importance in today’s society regarding different economic, environmental, and social challenges manifests itself in such as the increasing shortages of energy and water resources, high energy prices, ever-increasing energy demands and dependency on fossil fuels, and growing environmental concerns, due to decreasingly unsustainable humans’ lifestyles over recent decades. Human-induced global climate change and global warming are, in general, recognised as the greatest environmental threats (Raupach and Canadell, 2010). These concerns have led to the consideration of alternative and renewable energy sources (RES). Developing clean RES ranks as one of the greatest challenges facing mankind in the medium- to long-term (Mata et al., 2011). No single energy technology or combination of technologies exists that can address all challenges in a sustainable manner (Ma et al., 2011). A review (Wenzel, 2009) showed that the maximum available potential of biomass for energy purposes is around 10 – 50 % of fossil fuel substitution.

Biomass and bioenergy are widely considered as contributors to sustainability (Thornley et al., 2009). Biomass is one of the RES having increasing importance (Rentizelas et al., 2009) and from which heat, electricity, and biofuels can be generated (Lam et al., 2010) in a near carbon-neutral manner. CO_2 emitted during biomass combustion is namely absorbed during the biomass growth. Its utilisation can also improve energy security and independence, as well as the development of rural regions and employment.

The transportation sector relies almost exclusively on petroleum-based fuels, and about 30 % of the world’s fossil fuel consumption is related to transport. The reduction of fossil energy reserves and the associated environmental impact are the two main reasons that lead to considering the use of alternative fuels within the transportation sector (Jungbluth et al., 2007). In the short-term only biofuels from biomass could provide an alternative that can be implemented because of its high density, compatibility of current automobile engines, and existing fuels’ distribution infrastructures. Thus, bioethanol and biodiesel have become the more promising alternatives (Martín and Grossmann, 2013).

One of the more important long-term goals of the European Union (EU) in the field of energy is achieving self-sufficiency by oil and gas independent energy supplies with minimum emissions and waste produced. The EU has set ambitious targets for a transition to renewable energy. EU Member States are committed to achieving a 20 % share of renewable energies within the overall energy consumption of the EU, 20 % improvement in energy efficiency, and 20 % greenhouse gas (GHG) emission reduction by 2020 (European Commission, 2009). This directive also requires that each Member State ensures that the share of energy from renewable sources in all forms of transport in 2020 is at least 10 % of the final consumption of energy regarding transport in that Member State (European Commission, 2009). The contribution of biofuels towards these targets is expected to be significant (European Commission, 2012).

In the United States (US) also, the Federal Government approved Renewable Fuels' Standards (RFSs), such as Energy Policy Act of 2005 (109th US Congress; Public Law 109-58, 2005) and Energy Independence and Security Act (EISA) of 2007 (110th Congress; Public Law 110-140, 2007). Several US States have also adopted Renewable Portfolio Standards (RPS) legislation. EISA established minimum annual volume requirements, and minimum GHG emission reduction targets for several categories of renewable fuels that must be sold by producers and importers of petroleum-based transportation (Rubin and Leiby, 2013). EISA requires increasing the total amount of renewable fuels to be blended into transportation fuel to 36 billion US gallons by 2022, of which no more than 15 billion US gallons can be derived from corn starch (Faulkner, 2012). RPS is a regulation that requires the increased production of biopower from RES. It calls for approximately 11 % of the national electricity to be generated by renewable sources in 2030 (Jeffers et al., 2013).

In China, the Chinese government's law on renewable energy from 2006, indicated that biofuels from renewable sources would account for 5 % of the primary energy by 2010, and 10 % by 2020 (Chen and Qiu, 2010). Similar goals for the increase of bioenergy are set also in several other countries, such as India, Thailand, Mexico, Argentina and others (Faulkner, 2012).

Over the last few years there has been increasing criticism of first generation biofuels especially (Wetterlund et al., 2012). The first generation of biofuels, based on starch, sugar, and oil crops brought about an ethical trade-off, since the raw material could also be used for food, which may result in an increase in food prices and, eventually, supply risks (Ajanovic, 2011). An increase in cultivated fields may lead to biodiversity loss, due to the conversion of land not currently in crop production, such as forest and grassland (Mata et al., 2011). Consequently, second and third generations have been proposed as a solution in order to improve the yields, reduce the consumption of utilities during the production process, whilst using a raw material that does not compete with food (Čuček et al., 2011b). It should be noted that the production of 2nd and 3rd generation biofuels is not yet commercial, although the pilot and demonstration facilities are being developed (Naik et al., 2010). In order for the biofuel industry to be competitive with petroleum-based fuels, as well as providing further benefits, a more profitable, better integrated, and more sustainable biorefinery supply network design is crucial for attracting investments towards the production of more sustainable biofuels (Čuček et al., 2012d). Thus, the competitiveness of biomass as an energy source faces some important challenges (Čuček et al., 2012d). It strongly depends on the biomass supply chain (Yu et al., 2009) due to expensive logistics (Gnansounou, 2011). Biomass is usually seasonally and locally available, has low energy density and high moisture content, degrades during storage, and requires extensive infrastructure for harvesting, transportation, storage, and processing (Lam et al., 2010). All these operations are energy-intensive, and if not performed on the appropriate scale and sequence may result in unacceptably high costs and GHG emissions

(Čuček et al., 2010). The production of bioproducts should be based only on sustainable pathways (Scott et al., 2012).

Indicators measuring sustainable development (SD) are of paramount importance in ensuring SD (Ng et al., 2012). Many different concepts and methods have already been developed for the environmental, economic, and social evaluations of particular processes, products or activities (Jeswani et al., 2010), such as Life Cycle Assessment (LCA), Social LCA (SLCA), ecological footprint, and many others. Different indicators of SD have been presented in various sources, journal papers, e.g. (Čuček et al., 2012c), books, e.g. (Hák et al., 2007), publications of different organisations, such as International Atomic Agency (International Atomic Energy Agency, 2005), United Nations (United Nations, The Department of Economic and Social Affairs, 2007), and many others. Amongst the developed indicators footprints (Čuček et al., 2012c), sustainability indexes (Azapagic et al., 2002) and combined criteria, such as eco-cost (Vogtländer et al., 2010) and eco-profit (Čuček et al., 2012a) play important role.

Paving the way towards sustainability and SD that should encompass the integration of economic, environmental, and social components at all levels (Čuček et al., 2012c), leads to a complex multi-objective optimisation (MOO) problem (Fu et al., 2000). Processes, technologies, products, or activities should be economically-viable, environmentally-benign, and socially-just, in order to be more sustainable. As these desired qualities often represent conflicting targets, simultaneous MOO must be performed in order to obtain compromise solutions (trade-offs) that reveal the possibilities for achieving improvements within the system (Azapagic and Clift, 1999). MOO problems should be solved optimally by preventing subjective steps as much as possible (Kravanja and Čuček, 2013). MOO should even deal with uncertainty because of scarce and uncertain data (Fu et al., 2000).

Important limitations in the case of considering more evaluated objectives are computational burden (Guillén-Gosálbez, 2011), time consumption, difficulty regarding visualisation and interpretation of the objective space (Deb and Saxena, 2005), and providing only the narrow views of two, three or; at most; four dimensional (4-D) Pareto projections (Čuček et al., 2013a). Reduction of the dimensionality is thus required. Reduction and aggregation of different objectives have so far mostly relied on the decision-makers' preferences. Yet, it should be based on a systematic mathematical approach (Guillén-Gosálbez, 2011).

1.1 Outline of the Thesis

This thesis contains seven parts, i) Introduction, ii) Theoretical Backgrounds, iii) Integrated Synthesis of Bioethanol Production from the Entire Corn Plant, iv) Synthesis of a Regional Network for the Production of Biomass Products, v) Assessment Methods for Sustainable Development Within Multi-Objective Optimisation, vi) Reducing the Dimensionality of the Criteria in Multi-Objective Optimisation, and vii) Conclusions and Future Work. This thesis is comprised of two main categories: i) synthesis of bioprocesses and supply networks and ii) inclusion of sustainability metrics in order to synthesise sustainable bioprocesses and supply chain networks.

After the introduction provided in this Chapter, the following Chapter 2 provides theoretical backgrounds to mathematical programming (MP), including the single-objective optimisation (SOO), and MOO, the production of biomass for bioproducts, focusing particularly on biofuels' production, biomass supply chain networks, assessment methods for the evaluation of SD, and methods for dimensionality reduction of criteria.

Chapter 3 presents the synthesis of an integrated process of bioethanol production from the entire corn plant in terms of raw material (corn grain and stover), technologies (they are shared between processes), and energy (excess energy from one process is integrated with another process which needs energy). Different process technologies are considered, such as biochemical, thermo-chemical and thermo-biochemical processes, and the first- and second-generation ethanol production. This work was published in (Čuček et al., 2011b) and an abridged version was presented in (Čuček et al., 2011c). The author of this PhD thesis was partially responsible for modelling the integrated process, case study formulation, optimisation, and for analysing the results. The author is the first author of these contributions, and wrote significant parts of them.

Chapter 4 is an extension of synthesising integrated processes to the synthesis of regional networks by considering the competition between fuels and food production. Regional supply chain networks are divided into four layers: supply zones (agricultural layer), a collection, storage and pre-processing layer, a processing layer, and a demand layer. Two syntheses of regional networks for the production of biomass products are considered, simplified, and more comprehensive multi-period synthesis. Simplified synthesis is presented in detail in (Lam, 2010), and is therefore only presented in short in this dissertation. Multi-period synthesis is described in this thesis in more details. In comparison with the simplified model it includes several additional features, such as accounting for seasonality and the availability of biomass resources, enabling the recycling of products, includes Total Site (TS) heat integration (HI), and others, in order to be even more useful for real-world applications and decision-making. Simplified synthesis of regional networks is illustrated regarding the different biomass energy supply chains, and a more comprehensive synthesis regarding the regional biorefinery's supply networks including first, second and third generations of biofuels. Simplified synthesis was published in (Čuček et al., 2010), in which the author was responsible for the modelling and optimisation of the supply-network synthesis, and partially responsible for the case study formulation, data collection and for analysing the results. Multi-period synthesis is planned to be published in (Čuček et al., 2013c), and an abridged version has been accepted for publication in (Čuček et al., 2013b). The author was responsible for the mathematical multi-period synthesis model formulation and for the research process, and partially responsible for data collection, and for analysing the results. The author wrote significant parts of those contributions relating to the synthesis of regional supply chain networks.

Chapter 5 presents several methods for evaluating the sustainability and SD of process technologies and entire supply chain networks. Different assessment methods for measuring SD are presented: i) footprints, ii) sustainability indexes, and iii) eco- and total profits, and other combined criteria. All the sustainability metrics are used within MOO, and besides the direct, also consider the indirect and total effects on the environment, which represent new advanced SD measuring concepts by also considering the unburdening of the environment. Assessment methods are presented on illustrative examples of regional biomass and bioenergy networks, and on the biogas production supply chain. The work dealing with direct, indirect, and total footprints is published in (Čuček et al., 2012a), and the shortened version in (Čuček et al., 2011a). The author was responsible in these two works for data collection and the research process, and partially responsible for analysing the results. Sustainable synthesis of biogas processes using the concept of eco-profit is published in (Čuček et al., 2012a) where eco-profit was introduced, and in (Kravanja and Čuček, 2013) where eco-profit was further extended. The responsibility of the author lay in optimising the sustainable biogas production supply chain, and also partial responsibility relating to the data collection and analysing of the results. MOO when considering total effects, total profit and total sustainability index, was published in (Kravanja and Čuček, 2013), where the author was responsible for modelling, case study formulation and optimisation, and partially responsible for data collection, and the analysing of the results. The author wrote significant parts of those contributions relating to evaluating the sustainability and SD of regional supply chain networks.

Chapter 6 deals with the systematic reduction and aggregation of different objectives within MOO problems. A novel dimensionality reduction method is presented, a Representative Objectives Method (ROM), by which the number of footprints (or any other criteria) is reduced to a minimum number of representative ones. The number of footprints is reduced through similarities amongst those footprints that show similar behaviour. It has so far been applied to environmental footprints and cases where the models are known. ROM is illustrated using an illustrative example of different biomass energy supply chains. This approach makes MOO more practical for real-life problems and decision-making. This part of the work dealing with ROM was published in (Čuček et al., 2013a). The author's contribution to this work was the case study formulation and optimisation, and partially the data collection, analysing of the results, and writing the scientific contribution.

The concluding Chapter 7 presents the summary of the research work presented in this thesis. This is then followed by recommendations for future research within this field.

2 THEORETICAL BACKGROUNDS

This Chapter provides the theoretical background. First the MP is described, then an introduction to the synthesis of biofuels and bioproducts production. Biofuels and bioproducts were widely considered several years ago as contributors to sustainability (Thornley et al., 2009). However, some questions about their sustainability have arisen over recent years (Zamboni et al., 2011), especially relating to food production and prices (Ajanovic, 2011), the safety of food supplies, and biodiversity loss (Mata et al., 2011), water depletion, nitrogen footprint (NF) (Čuček et al., 2012b), phosphorus usage (Ashley et al., 2011), etc.

It was because of the above mentioned reasons, that progress to sustainability and SD have to be evaluated, and should be based on LCA and within MOO. The life cycle scope should be considered in order to avoid problem shifting (Finnveden et al., 2009), and simultaneous MOO must be performed in order to obtain compromise solutions amongst different objectives, such as technical, economic, environmental, and social.

2.1 Mathematical Programming

MP is also called ‘mathematical optimisation’, or ‘optimisation’. Optimisation is the use of specific methods for determining the best solutions to the problem or design of a process, subject to given constraints. It is the act of obtaining the best result under given circumstances (Rao, 2009). A wide-variety of problems throughout chemical engineering and other fields can be resolved by optimisation (Edgar et al., 2001). Optimisation techniques are being used over a wide spectrum of industries, including aerospace, automotive, chemical, electrical, construction, and manufacturing industries (Rao, 2009). The typical problems in chemical engineering arise during process design, process control, model development, process identification, and real-time optimisation (Biegler, 2010). The sizes and complexities of the problems that can be solved using optimisation techniques are also increasing due to the rapidly advancing computer technology (Rao, 2009). Optimisation is the key methodology used for sustainable process design and synthesis (Klemeš et al., 2010).

The first step when setting out to optimise any system is to identify the objective to be maximised or minimised: the criterion to be used for judging the system’s performance. In regards to a chemical process, the main objective for most companies is to maximise profits (Sinnott, 2005). There are also other sub-objectives, such as minimising the operating cost, maximising the product yield and so on. The values of the objective function are determined by manipulation of the problem’s variables, which represent discrete and continuous variables that are allowed to vary within a certain range, and those parameters the values of which do not vary.

The general form of the mathematical programming is the mixed-integer non-linear program (MINLP), which takes the following form:

$$\begin{aligned} \min_{x,y} \text{ or } \max \quad & \boldsymbol{c}^{\mathrm{T}}\boldsymbol{y} + \boldsymbol{f}(\boldsymbol{x}) \\ \text{s.t.} \quad & \boldsymbol{h}(\boldsymbol{x},\boldsymbol{y}) = 0, \\ & \boldsymbol{g}(\boldsymbol{x},\boldsymbol{y}) \le 0, \\ & \boldsymbol{x} \in \boldsymbol{R}^{n}, \ \ \boldsymbol{y} \in \{0,1\}^{m} \end{aligned} \tag{2.1}$$

where $\boldsymbol{x}$ denotes a vector of involved continuous variables (flow-rates, design variables, etc.), whilst $\boldsymbol{y}$ is the vector of involved binary decision variables or discrete decisions (existence of particular stream, process unit, technology, etc.). Function $\boldsymbol{f}(\boldsymbol{x})$ is objective function to be minimised or maximised (profit, cost, energy consumption, etc.). The equality constraint $\boldsymbol{h}(\boldsymbol{x},\boldsymbol{y}) = 0$ denotes the equations that describe the performance of the system (mass and energy balances, design equations, etc.). The inequality constraints $\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y}) \le 0$ can define process specifications or constraints (product specifications, environmental constraints, etc.).

Problem (2.1) corresponds to an MINLP when any of the functions involved are non-linear. If the functions $\boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{h}(\boldsymbol{x},\boldsymbol{y})$ and $\boldsymbol{g}(\boldsymbol{x},\boldsymbol{y})$ are linear, then problem (2.1) corresponds to a mixed-integer linear program (MILP). If all the variables are integer, this gives rise to an integer programming (IP) problem. If there are no binary (0/1) variables, the problem (2.1) reduces to the non-linear program (NLP) or linear program (LP) (Biegler, 2010).

During this research work MILP, NLP, and MINLP problems were performed. An MILP problem was formulated for the synthesis of regional biomass energy supply chain networks (Čuček et al., 2010), for the multi-period synthesis of a biorefinery's supply networks (Čuček et al., 2013b), and for the sustainable synthesis of biogas processes (Čuček et al., 2012a). NLP problems were developed for two syntheses of ethanol and food production from the entire corn plant, one per alternative technology of processing the corn stover (Čuček et al., 2011b). The MINLP problem was employed for the two-level synthesis of sustainable bioethanol processes including different raw materials and technologies (Čuček and Kravanja, 2010), within an alternative formulation for the synthesis of regional biomass energy supply chain networks (Čuček et al., 2010), and within the sustainable synthesis of biogas processes (Čuček et al., 2012a) including non-linear terms.

Furthermore, the MP problems could be divided into steady-state (one-period) and dynamic (multi-period) systems. Several decisions involve multiple time periods (Ragsdale, 2007). Multi-period systems are systems where e.g., capacities, costs, demands etc. vary from period to period due to market, seasonal and other changes (van den Heever and Grossmann, 1999). Examples include almost all production systems, such as utility systems, refineries (van den Heever and Grossmann, 1999), hydrogen networks (Ahmad et al., 2010), biomass supply chain networks etc.

The generalised form of the multi-period model with time periods $tp \in TP$ is presented in (2.2):

$$\begin{aligned} \min_{x,y} \text{ or } \max \quad & \boldsymbol{c}^{\mathrm{T}}\boldsymbol{y} + \sum_{tp \in TP} \boldsymbol{f}_{tp}(\boldsymbol{x}_{tp}, \boldsymbol{d}) \\ \text{s.t.} \quad & \boldsymbol{h}_{tp}(\boldsymbol{x}_{tp}, \boldsymbol{d}, \boldsymbol{y}) = 0, \\ & \boldsymbol{g}_{tp}(\boldsymbol{x}_{tp}, \boldsymbol{d}, \boldsymbol{y}) \le 0, \\ & \boldsymbol{g}_{tp}^{\mathrm{D}}(\boldsymbol{x}_{tp}, \boldsymbol{y}) \le \boldsymbol{d} \\ & \boldsymbol{x}_1 = \boldsymbol{x}_{|\boldsymbol{T}|} \\ & (\boldsymbol{x}_{tp}, \boldsymbol{d}) \in \boldsymbol{R}^n, \ \boldsymbol{y} \in \{0,1\}^m \end{aligned} \tag{2.2}$$

where continuous variables $\boldsymbol{x}$ and constraints $\boldsymbol{f}, \boldsymbol{g}, \boldsymbol{h}$ are indexed by *tp*, whilst design variables $\boldsymbol{d}$ (unit sizes) are not. Constraint $\boldsymbol{g}_{tp}^{\mathrm{D}}(\boldsymbol{x}_{tp}, \boldsymbol{y}) \le \boldsymbol{d}$ defines that the value of the design variable should be greater than or equal to the maximal value of continuous variable from each time periods *tp*. $\boldsymbol{x}_1 = \boldsymbol{x}_{|\boldsymbol{T}|}$ represents the continuity equation which means circular operation in time, the first time period follows after the last one (Sousa et al., 2008).

Depending on the number of objective functions to be maximised or minimised, optimisation problems can be classified as SOO or MOO problems.

2.1.1 Single- and Multi-Objective Optimisation

SOO is an important special case of an optimisation problem with only one objective function. A single optimal solution is obtained. SOO has the advantage of its simplicity, and the providing of decision makers with insights into the nature of the problem (Savic, 2002).

However, many real-world decision-making problems need to achieve several objectives, such as maximising the energy efficiency, maximising the profit, minimising the environmental burden, etc. MOO, also known as multi-criteria, vector, multi-attribute and Pareto optimisation, and multi-objective programming (Wikipedia, 2013), simultaneously integrates two or more objectives or goals that are subject to certain constraints. Usually compromise solutions (trade-offs) are obtained that reveal the possibilities for achieving improvements within the system (Azapagic and Clift, 1999). In general, no single solution exists where all the objectives are optimised simultaneously, but a number of Pareto optimal solutions (a feasible region of optimal solutions, Pareto front) is obtained (Rao, 2009).

Several methods have been developed for solving MOO problems. The simplest method is to transform the MOO problem into a SOO problem by applying weights to different criteria (the weighted objective method). Other widely used optimisation methods are the ε-constraint method (Haimes et al., 1971), in which a sequence of constrained single-objective problems is solved; the goal-programming method, in which the solution is obtained by minimising a weighted average deviation of the objective functions from the goal set by the decision-maker, and evolutionary algorithms that involve random search techniques (Bhaskar et al., 2000). The solution for such problems is a set of “non-inferior” or Pareto points (Čuček et al., 2012c).

Many tools have been developed for being helpful during optimisation. They offer formulating models in the forms of LP, NLP, MINLP, or other types of problem, and for numerically solving a certain optimisation problem. Amongst the tools for performing SOO or MOO are the General Algebraic Modelling System – GAMS (GAMS Development Corporation, 2010), A Mathematical Programming Language – AMPL (AMPL, 2011), Advanced Interactive Multidimensional Modelling System – AIMMS (Roelofs and Bisschop, 2011), the Mixed-Integer Process SYNthesizer – MIPSYN (Kravanja, 2010), and others. They support a range of different types of solvers for different types of models, such as BARON, GUROBI, CONOPT, CPLEX, DICOPT, MINOS, OQNLP, etc.

In this research work several MOO problems were solved and will be presented in the continuation. The main objective of most problems is maximising the economic profit, whilst also eco-cost, eco-profit, net profit, and total profit. Secondary objectives differ amongst approaches. The most used technique for dealing with MOO when considering LCA, is by applying the ε-constraint method (Pieragostini et al., 2012). Different approaches have been considered for the secondary objective: an approach based on the relative sustainability index, and a concept based on direct and total footprints.

GAMS, a high-level modelling system for MP and optimisation, and MIPSYN modelling system with advanced synthesising capabilities, were used during the research work.

GAMS was the first algebraic modelling language (AML), and is designed for modelling LP, NLP, MILP, MINLP, and other optimisation problems. It is tailored for complex and large-scale modelling. The user can change the formulation quickly and easily, and can change e.g., NLP to MINLP models. It has a large community of users from various backgrounds of engineering and science (Wikipedia, 2012b).

MIPSYN is especially designed for large process schemes and MINLP optimisation (Kravanja, 2010). It implements the modelling and decomposition (M/D) strategy developed by (Kocis and Grossmann, 1989) and the outer-approximation and equality-relaxation algorithm (OA/ER) by (Kocis and Grossmann, 1987). MIPSYN enables automated execution of simultaneous topology and the parameter optimisation of processes enabling the solutions of large-scale MINLP problems.

GAMS is used for the synthesising of supply-chain networks and for problems with only a few blocks of equations and variables. Larger-scale and more complex process schemes are solved using MIPSYN.

2.2 Biofuels and Bioproducts Production

A growing population and the climate change are having an impact on increasing competition for land, energy, water, and biomass types for food and feed production, non-food usage – bioproducts, such as timber, cotton, paper, etc., and bioenergy – biofuels, such as bioethanol and fuelwood, heat, electricity, etc. (Wirsenius, 2007). Biofuels' production is expected to rise significantly because of government support in several countries, as well as higher petroleum prices. This sector has proved to be the largest source of new demand for agricultural land, and is affecting cereal prices (Food and Agriculture Organization of the United Nations, 2012).

Biofuels include fuels derived from biomass conversion, and can be solid, liquid, and gaseous. Amongst the solid biofuels are fuelwood, wood chips, pellets, animal dung, agricultural waste, charcoal, non-food energy crops, and others. Liquid biofuels comprise bioethanol, biodiesel, green diesel, green gasoline, pyrolysis oil, biopropanol, and others. Gaseous biofuels are biogas, landfill gas, syngas, propane, butane, uncompressed hydrogen, and others.

A major part of this research work dealt with liquid biofuels for transport, which are currently gaining in importance. Amongst the biofuels more widely produced are bioethanol and biodiesel. Bioethanol is mainly produced in the US and in Brazil, while it is biodiesel in the EU. In 2011, worldwide bioethanol production reached 84.6 GL, a slight decrease from 2010 when 87.1 GL of bioethanol was produced (Renewable Fuels Association (RFA), 2013). Biodiesel production in 2010 rose to approximately 20 GL, with a 12 % increase from 2009 (Next Big Future and Z_1 Consulting Inc, 2011), when the global biodiesel production amounted to 17.9 GL (Biofuels Platform, 2010). In 2009 biofuels provided 2.7 % of the world's fuels for road transport (Next Big Future and Z_1 Consulting Inc, 2011). Biofuels have the potential to provide 27 % of total transport energy by 2050 (International Energy Agency, 2011).

Other minor transportation fuels produced from biomass are biomethanol, biopropanol, biobutanol, biohydrogen, green diesel, Fischer-Tropsch (FT) diesel, biodimethyl ether, bio-oils, biomethane, and others.

2.2.1 Process of Biofuels Production

There are different biomass conversion processes, which are based on biological, chemical, thermal, physical, thermo-chemical conversion, and other combined conversions. The conversion routes are based on the characteristics of biomass feedstock, if it includes mostly starch, sugar, oil or lignocellulose. The main conversion technologies are dry- and wet-milling processes, hydrolysis, fermentation, transesterification, gasification, pyrolysis, catalytic synthesis, and anaerobic digestion (AD).

Biomass feedstock, conversion technologies of biomass to biofuels, produced biofuels, and the main by-products, are shown in Figure 2-1.

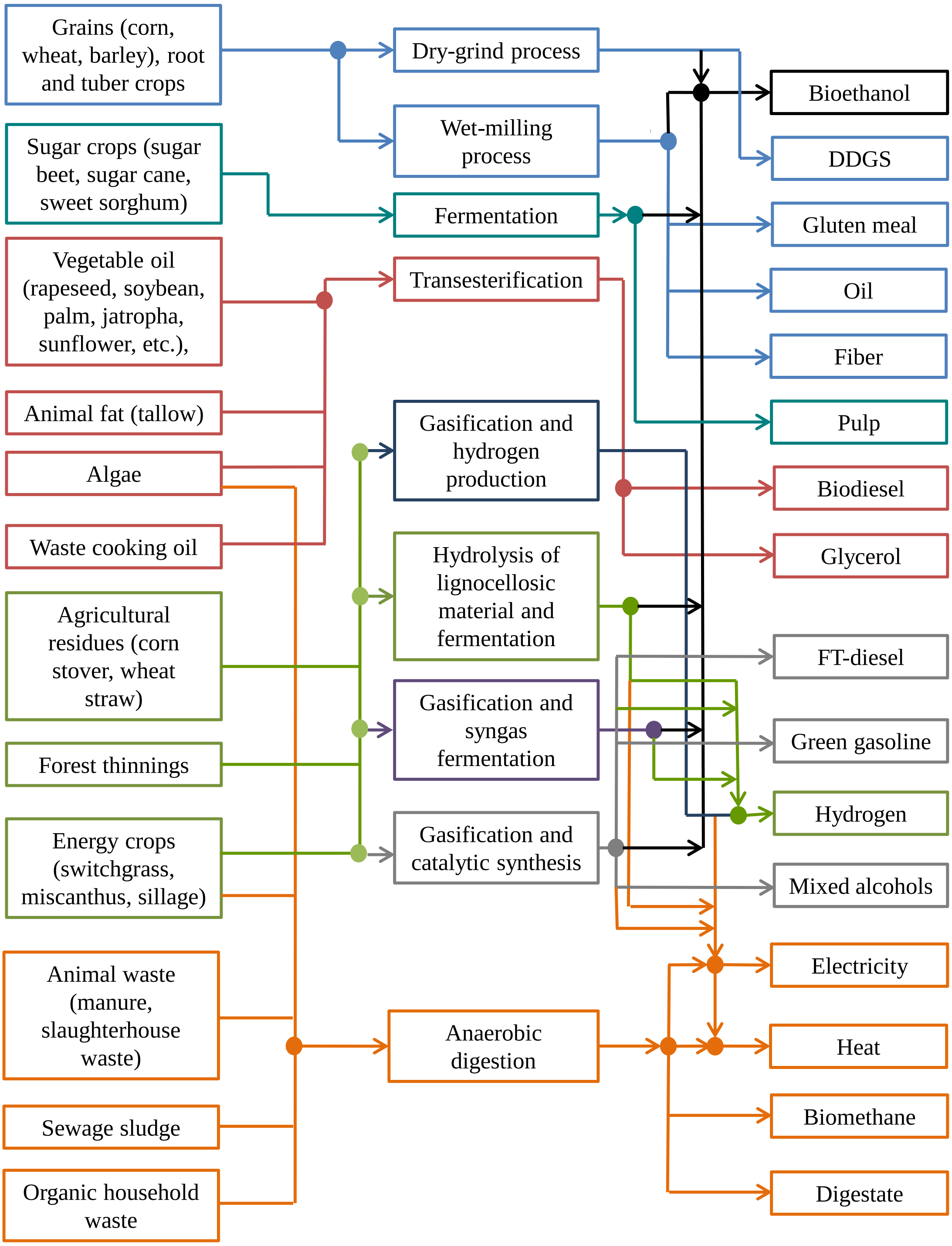


Figure 2-1. Biomass feedstock conversion technologies to biofuels and main by-products

Bioethanol is commercially produced from cereals, sugars, millets, and root and tuber crops (Speight, 2011). The common sugar crops are sugar cane, sugar beet, and sweet sorghum, and the more common starchy crops are corn, wheat, barley, potatoes, cassava, and others. The main advantage of using sugar crops is their high yield of sugar per area, and low conversion costs, however, their main disadvantage is their natural seasonal availability (Vertes et al., 2010). Most of the ethanol currently produced is via the dry-grind process and the wet-milling process converting starches to ethanol. Among those technologies the dry-grind process is prevalent, and much of the current expansions of the industry use this technology. The main difference amongst those processes is that starchy crops require the additional process of converting the starches into sugars prior to fermentation, and therefore there is a lower energy requirement when converting sugars to ethanol. The dry-grind and wet-milling processes differ in the treatment of the crop before fermentation, and in the resulting by-products. The wet-milling process is more complex and capital-intensive than the dry-grind process, but produces a range of products including oil, gluten meal, fiber, and ethanol (Prieler and Fischer, 2009). The dry-grind process produces only distillers dried grains with solubles (DDGS) besides ethanol.

The common feedstocks used in biodiesel production include vegetable oil (rapeseed, soybean, palm, jatropha, sunflower, and other oils), tallow, waste cooking oil, and algae. Base-catalysed transesterification is the more common method in the production of biodiesel and the main by-product glycerol. There are other methods, such as the acid-catalysed process, the enzyme catalysed process, the supercritical process, etc. Batch and continuous processes are currently operating, amongst them batch production is currently favoured, however continuous processes are expected to gain wider acceptance in the near future due to higher production capacities and lower operating costs (Helwani et al., 2009).

Second generation biofuels are produced by using lignocellulosic biomass, such as agricultural residues (corn stover, wheat straw), forest thinning, and energy crops, such as switchgrass, miscanthus, corn silage, grass, etc. There are three main routes for producing second generation ethanol, the thermochemical route, the biochemical route, and the thermo-biochemical route. The thermochemical route works at high temperatures in the absence or presence of oxygen, air, and steam. Hydrogen can also be produced via the thermochemical and thermo-biochemical routes when syngas is cleaned. Besides producing hydrogen, syngas can be either further fermented to ethanol or catalytically-synthesised to ethanol and mixed alcohols, such as propanol, butanol, and others. Alternatively, syngas can be catalytically-synthesised to FT-diesel and green gasoline.

Animal waste, such as manure, slurries, and slaughterhouse waste, as well as a wide range of digestible organic waste from dairy production, food industries, and agro-industries, sewage sludge, the organic fraction of municipal solid waste (MSW), organic waste from household and energy crops, can be converted through AD to biogas (from which heat and electricity or biomethane can be generated), and organic fertiliser (digestate). Also algal oil can be anaerobically-digested to produce biogas (Lundquist et al., 2010).

Several biofuel production technologies are applied within the illustrative examples. The dry-grind process, and gasification followed by either syngas fermentation or further catalytic synthesis are applied within Chapter 2. The dry-grind process, AD, MSW incineration, timber sawing and incineration are considered within Sections 4.1, 5.1.3, and Chapter 6. Several biofuel production technologies, such as the dry-grind process, gasification and further syngas fermentation, gasification and further catalytic synthesis, the biochemical process for lignocellulosic biomass, FT-diesel and green gasoline production, hydrogen production and biodiesel production are evaluated within Section 4.2.2, and AD within Sections 5.2.4 and 5.3.3.

2.3 Biomass Supply Chain Networks

The competitiveness of biomass as an energy source strongly depends on the biomass supply chain, from the land to the bioproducts' end use (Yu et al., 2009). Biomass is usually seasonally and locally available, has low energy density and high moisture content, and degrades during storage. The biomass supply chain includes growing, harvesting, transporting, pre-treatment, and pre-processing (such as densification, compacting, grinding, drying, extraction), storing, and the processing into bioproducts, and that requires an extensive infrastructure (Lam et al., 2010).

Supply chain usually consists of key 4 stages or layers:

i) Harvesting and supply layer (layer 1 – L1)
ii) Collection, and pre-processing layer (layer 2 – L2)
iii) Conversion layer (layer 3 – L3)
iv) Consumption layer (layer 4 – L4).

Transport, storage, and handling link the various layers to each other.

The generic structure of the supply chain consisting of four layers is shown in Figure 2-2.

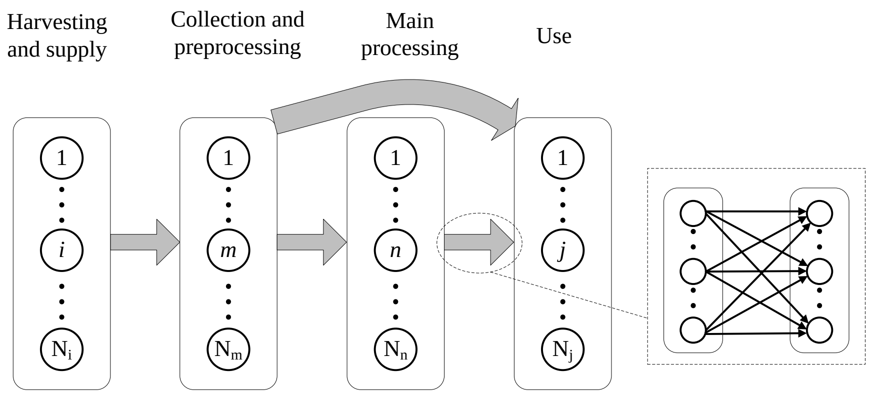


Figure 2-2. The generic structure of the supply chain (Čuček et al., 2010)

There are several critical issues to be addressed:

i) Availability of each raw material with respect to prices, quality, quantity and sustainability;
ii) Relatively high demand for water and nutrients by several biomass types;

iii) Reliability and continuity of biomass supply (poses challenge to storage, handling, and transportation);

iv) The choice of collection method, and the incorporation of the pre-processing into the supply chain can reduce the logistical cost;

v) High capital and running cost of biomass systems;

vi) Smaller-scale vs. larger-scale biomass processing;

vii) Selection of the most sustainable mode of transportation. Biomass is relatively expensive to transport. Pipelines, rail, and water transports are more sustainable, however over shorter distances (up to 500 km) road transport is preferable and cheaper (Searcy et al., 2007).

2.4 Evaluation of Sustainable Development

SD represents development that "meets the needs of the present without compromising the abilities of future generations to meet their own needs" (World Commission on Environment and Sustainable Development (WCED), 1987). SD requires an integration of economic, environmental and social components at all levels (Organisation for Economic Co-Operation and Development (OECD), 2004). Sometimes SD also incorporates a fourth dimension, an institutional (Herva et al., 2011) or a cultural (Nurse, 2006) component. Some authors have discussed more than four dimensions of SD. Five dimensions (Ilskog, 2008), or even seven (Perlas, 1994), have been cited, however they are rarely used. SD usually considers three dimensions or pillars ("triple bottom line"): environmental protection (ecology or planet), economic prosperity (profit), and social justice (people) (Organisation for Economic Co-Operation and Development (OECD), 2008). The three dimensions or pillars of SD are presented in Figure 2-3.

The goal of SD is to find a balance amongst these objectives. This search for a balance is the area within which the application of MP and other tools for sustainability evaluation can provide valuable support (Grossmann and Guillén-Gosálbez, 2010). MOO problems should be solved optimally by preventing subjective steps as much as possible.

Figure 2-3. Three pillars of sustainable development (Hecht et al., 2011)

In order to progress towards sustainability and SD, appropriate methods should be used for measuring sustainability and SD. The actual measurements of sustainability and SD remain an open question (Pozo et al., 2012). Indicators that can be used to measure SD need to be developed in order to provide a basis for decision-making. Many different concepts and methods have already been developed for the environmental, economic, and/or social evaluations of particular processes, products or activities (Jeswani et al., 2010), e.g., LCA, SLCA, Life Cycle Cost Analysis (LCCA), footprints, the environmental sustainability index, the measurement of net savings, eco-cost (Vogtländer et al., 2010), and others.

This research work implemented footprints, the environmental sustainability index, the extension of eco-cost to eco-profit, and other combined criteria. The footprints are applied within the illustrative example of a biomass energy supply chain (see Section 5.1), environmental sustainability index, and eco-profit, and other criteria within the illustrative example of an integrated process of biogas production (see Sections 5.2 and 5.3).

2.4.1 Life Cycle Assessment

Environmental indicators are usually defined on the basis of LCA (Pozo et al., 2012). LCA is a structured, comprehensive, internationally-standardised tool (environmental management standards ISO 14040 (International Organisation for Standardisation (ISO), 2006a) and 14044 (International Organisation for Standardisation (ISO), 2006b) for quantifying those emissions, resource consumption, environmental, and health impacts associated with processes, products or activities. LCA is commonly referred to as a "cradle-to-grave" analysis (Glavič and Lukman, 2007), as an open loop. It takes into account the system's full life-cycle: from the extraction and processing of resources through manufacturing, usage, and maintenance to recycling or disposal, including all transportation and distribution steps (Bojarski et al., 2009). Over recent years a "cradle-to-cradle" – or closed loop – perspective has been introduced, which attempts to reach 100 % utilisation of all types of waste (Haggar, 2007).

The comprehensive scope of LCA is useful in order to avoid problem-shifting, for example, from one phase of the life cycle to another, from one region to another, or from one environmental problem to another (Finnveden et al., 2009). LCA can help to reduce environmental pollution and resource usage, and often improves the profitability (McManus, 2010). LCA is an adequate instrument for environmental decision support and has gained wider acceptance over recent years within both academia and industry (von Blottnitz and Curran, 2007).

An LCA principle and framework is divided into four phases: Goal and Scope definition, Life Cycle Inventory (LCI), Life Cycle Impact Assessment (LCIA) and Interpretation. Those phases and direct application of LCA framework are shown in Figure 2-4.

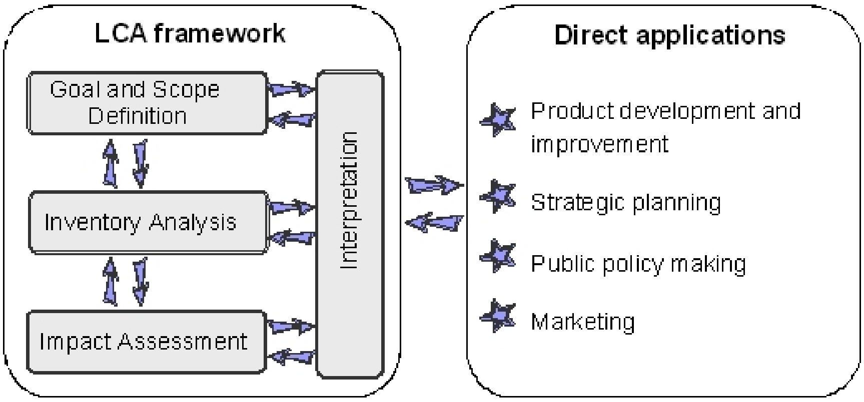


Figure 2-4. Four phases and direct applications of Life Cycle Assessment (European Commission; Joint Research Centre, 2013)

During the first phase the objectives of the analysis and the system's boundaries should be defined, such as functional unit, assumptions and limitations, allocation methods (when there are several products or functions of the system), and the chosen impact categories. The goals and scope can be adjusted during the iterative process of the analysis. The second phase involves data collection relating to inputs of materials and energy, and outputs including releases to air, soil, and water. All the data should be related to the functional unit defined at the first phase. The third phase of LCA is aimed at evaluating the significance of environmental impacts quantified in the LCI. The relative contribution of each environmental impact should be assigned to specific impact categories (global warming potential, acidification potential, carbon footprint (CF), NF, land usage, etc.). Other optional LCIA elements such as normalisation (comparing the results to e.g. population or area of Europe), grouping (sorting and ranking of impact categories), and weighting may also be conducted. Weighting, however brings a high degree of subjectivity into LCA analyses. Interpretation is the last phase of the LCA analysis, which should evaluate the study in a systematic way by considering its completion, consistency, and sensitivity analysis. Interpretation should also identify areas that have the potential for improvement within a system, and draw conclusions and recommendations.

LCA methodology and sustainability assessment, in general, still has certain major limitations that need to be overcome. The main limitation is the high degree of uncertainty arising from the LCI, which gives rise to results with high variability. Data quality and quantity is often insufficient for a comprehensive LCA. A possible consequence of discrepancies in data is that two independent studies analysing the same products may generate very different results, and also different LCIA methodologies can yield different results (McManus, 2010). Another limitation is the lack of a systematic method for generating and identifying sustainable solutions (Grossmann and Guillén-Gosálbez, 2010). There is no single method that is universally acceptable (Hendrickson et al., 1997). It is very challenging to define indicators that are not too broad or too specific (De Benedetto and Klemeš, 2010). Performing the LCA analyses can be costly regarding data, resources, and be time-intensive.

2.5 Dealing with the High Dimensionality of Criteria

SD should encompass the integration of economic, environmental, and social components at all levels, and thus require complex MOO. Compromise solutions (trade-offs) are obtained that reveal the possibilities for achieving improvements within the system (Azapagic and Clift, 1999).

One of the common ways of presenting the criteria is by plotting them on a spider diagram (Shonnard et al., 2003). Often, the number of different objectives is reduced by aggregating them within an aggregated single sustainability indicator, using the weighted sum method (Zadeh, 1963), the geometric mean of the applied indicators' ratios (Sikdar, 2007), the Sustainable Environmental Performance Indicator (SEPI) (De Benedetto and Klemeš, 2009), the Sustainable Process Index (SPI) (Krotscheck and Narodoslawsky, 1996), and the Waste Reduction (WAR) Algorithm (Hilaly and Sikdar, 1994), to name but a few. However, all approaches, even these, have some drawbacks. One of them is that the weighted sum methods are based on subjective weighting and possible difficulty when selecting the best solution. The SPI and SEPI have difficulties, as ecological footprints, when converting them to be expressed as area units. Optimising aggregated metrics in MOO has the effect of leaving some optimal solutions out of the analysis (Vaskan et al., 2012).

For simplicity, just one or two objectives have been considered during several studies (Guillén-Gosálbez, 2011). Yet, more realistic solutions could be obtained if more impacts were to be considered (e.g., economic performance and several environmental footprints). However, there are several limitations. An important limitation is that the computational burden increases rapidly in size with the number of objectives (Guillén-Gosálbez, 2011). Other limitations are that MOO can be time consuming, and there are often difficulties when visualising and interpreting the objective spaces (Deb and Saxena, 2005). It also prevents the carrying-out of an exact optimisation, resulting in only two, three; or at most; 4-D Pareto projections, thus providing only a narrow view when producing underestimated environmental metric estimates (Kravanja, 2012). Reduction of the MOO dimensionality is thus required, without compromising the qualities of the Pareto solutions.

The reductions and aggregations of different objectives have so far mostly relied on the decision-makers' preferences (Guillén-Gosálbez, 2011). Yet, it should be based on a systematic mathematical approach. Various dimension reduction approaches have been developed for this purpose that are generally categorised into linear and non-linear methods (Lygoe, 2010). The more-widely used linear methods are Principal Component Analysis (PCA) and Factor Analysis, which are second-order methods, i.e. rely only on information contained within the covariance matrix (Lygoe, 2010). Amongst the higher-order linear methods are Projection Pursuit, and Independent Component Analysis. Different methods are also used in the case of non-linearity, such as Non-Linear PCA, Non-Linear Principal Curves, Multi-D Scaling, Topologically Continuous Maps and Vector Quantisation. The review of the different methods was made by Lygoe (Lygoe, 2010).

This dissertation presents a novel dimensionality reduction method, a ROM (see Chapter 6), by which the number of objectives (footprints) is reduced to a minimum number of representative ones through similarities amongst those footprints that show similar behaviour. The ROM is illustrated using an illustrative example of different biomass energy supply chains.

3 INTEGRATED SYNTHESIS OF BIOETHANOL AND FOOD PRODUCTION FROM THE ENTIRE CORN PLANT

This Chapter proposes the integrated design of a biorefinery that is capable of fully using the entire corn plant, the dry-grind process and gasification technologies. The aim of this part of the work is to optimise the integrated biorefinery that uses corn grain and stover in such a way that equipment can be shared and the energy can be integrated. Two technological routes are proposed depending on the technology for processing corn stover. Corn grain is processed into ethanol using the dry-grind process (Karuppiah et al., 2008), and corn stover using the gasification and further syngas fermentation or catalytic synthesis (Martín and Grossmann, 2011a). The integrated technology enables lower investment cost, HI between the process with energy demand (the dry-grind process) and the process with excess of energy (thermo-processes), lower water consumption, and decreased usage of agricultural land compared to two separated technologies.

3.1 Superstructure

Firstly, the superstructure of the integrated process of bioethanol production from corn grain is postulated using the dry-grind process (biochemical process) and corn stover using two gasification routes, gasification and further syngas fermentation (thermo-biochemical process) and gasification and further catalytic synthesis (thermo-chemical process). The problem is decomposed into two subproblems, one per alternative technology for processing corn stover. The proposed general superstructure of the integrated process is shown in Figure 3-1. The integration begins with the use of the raw material (entire corn plant).

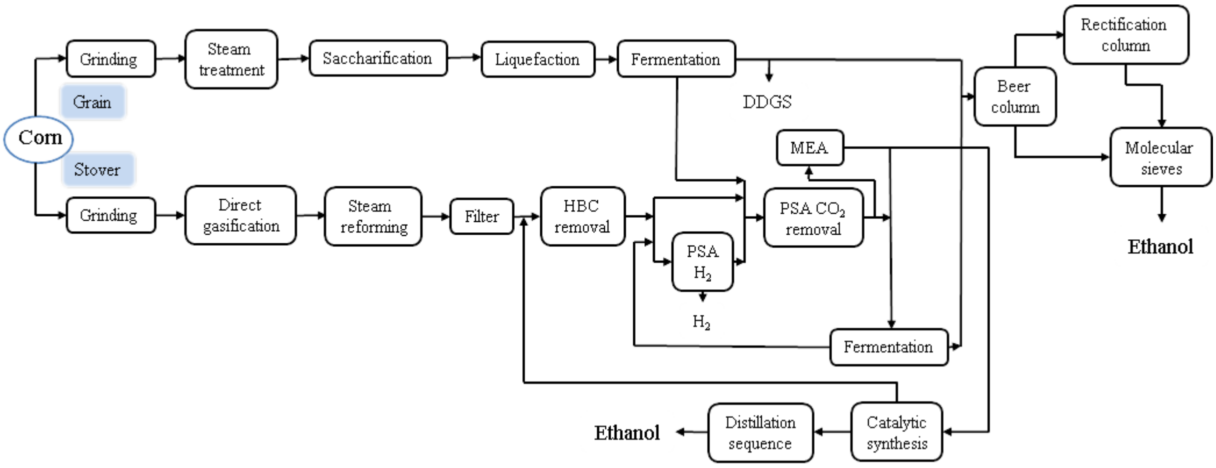


Figure 3-1. General superstructure of the integrated process (modified from (Čuček et al., 2011b))

The grain follows the dry-grind process path (see Figure 3-2). First, the corn kernels are washed and ground into flour. The formed ground flour structure is broken by steam treatment to form a mash. Enzymes are added to liquefy starch to maltose and further to produce glucose. The formed sugars are fermented towards ethanol, CO_2, acids and other minor by-products by using yeast strain *Saccharomyces cerevisiae*. The solids and liquids are separated before the beer column. The ethanol is concentrated and purified in distillation columns, corn grits, and molecular sieves to fuel quality ethanol with purity ≥ 99.5 wt%. The wet solids are pressed, combined with the recovered proteins, and dried. A by-product, DDGS is obtained that can be sold as cattle feed, thus contributing to the economics of the process. Further details of the units' models can be found in (Karuppiah et al., 2008).

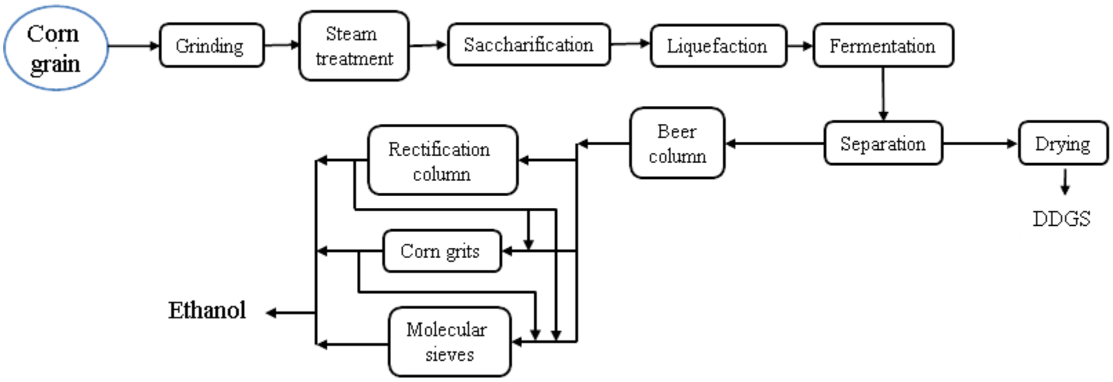


Figure 3-2. The dry-grind production process (modified from (Čuček et al., 2011b))

Corn stover follows either gasification and further syngas fermentation or gasification and further catalytic synthesis path (see Figure 3-3).

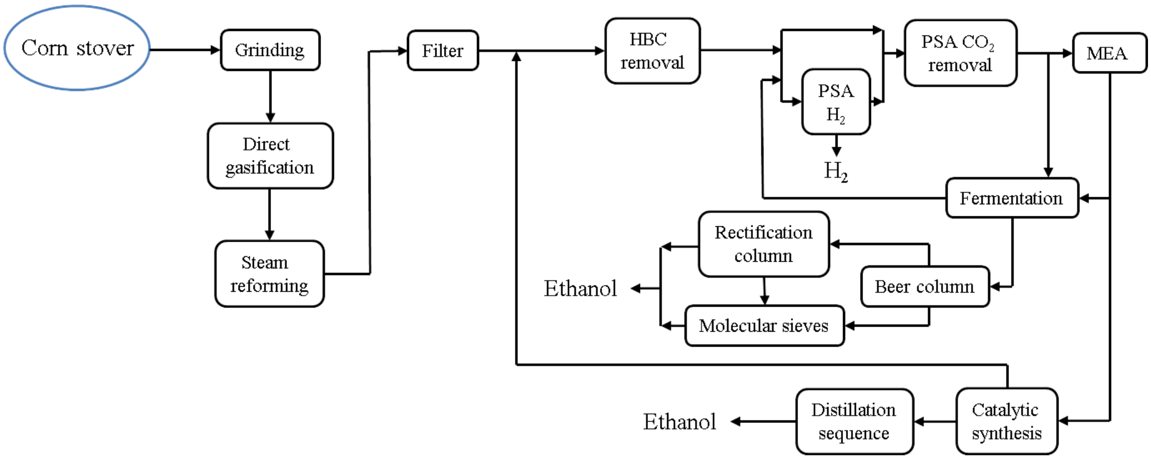


Figure 3-3. Combined thermochemical and thermo-biochemical ethanol production process (modified from (Čuček et al., 2011b))

Corn stover is treated using high pressure direct gasification with steam and oxygen. The gas is cleaned from solids and chemicals over a series of stages. Firstly, the char is removed using a cyclone. Next, the hydrocarbons are reformed with steam, and gas is purified following the hot-cleaning technology based on filters. Traces of hydrocarbons (HBC) are removed within a Pressure Swing Adsorption (PSA) system. The composition of the syngas is adjusted, so that the molar ratio CO : H_2 becomes 1 using a hybrid membrane – pressure swing adsorption (PSA) system. Hydrogen is produced, which importantly contributes to the economics of the process. Next, sour gases, such as CO_2 and H_2S, are removed from the stream using a combined technology, PSA adsorption, which mainly removes CO_2, and absorption on monoethanolamines (MEA), which can also remove H_2S depending on the synthetic path.

Two synthetic paths are proposed, the fermentation of the syngas towards ethanol (gasification and syngas fermentation) and the catalytic production of alcohols (gasification and catalytic synthesis). The H_2S is poisonous for the catalysts and must be removed, while the bacteria used can handle concentrations below 2.5%. By using the fermentation path, the diluted ethanol solution is dehydrated using the same technologies as in the dry-grind process, and therefore technologies are shared. In the case of using the catalytic path, a mixture of alcohols is produced, mainly methanol, ethanol and propanol, which is separated using a sequence of distillation columns.

These processes are modelled within the process simulator MIPSYN using mass and energy balances, and conversion constraints. The detailed superstructure which is used within MIPSYN is presented in Figure 3-4.

3.2 Integration of the Process

This part of the work presents the simultaneous integration of technologies, energy, and raw materials, in order to optimally produce ethanol.

The integration begins with the use of the raw material (corn grain and stover). It is assumed that from the entire plant around 50 % is grain and 50 % stover (Nelson, 2002). Corn stover harvest of 60 % is taken into account in order to keep the soil protected from erosion (Atchison and Hettenhaus, 2003). The typical flow of 18 kg/s of grain (Karuppiah et al., 2008) and 10.8 kg/s of stover are used as a base case for the optimisation.

Next, the technologies are shared, such as the same dehydration path for the biochemical and thermo-biochemical processes, as well as the carbon capture process units. However, if the biochemical and thermochemical paths are selected, the two processes would have to run in parallel, where the only common part is the technology for CO_2 capture.

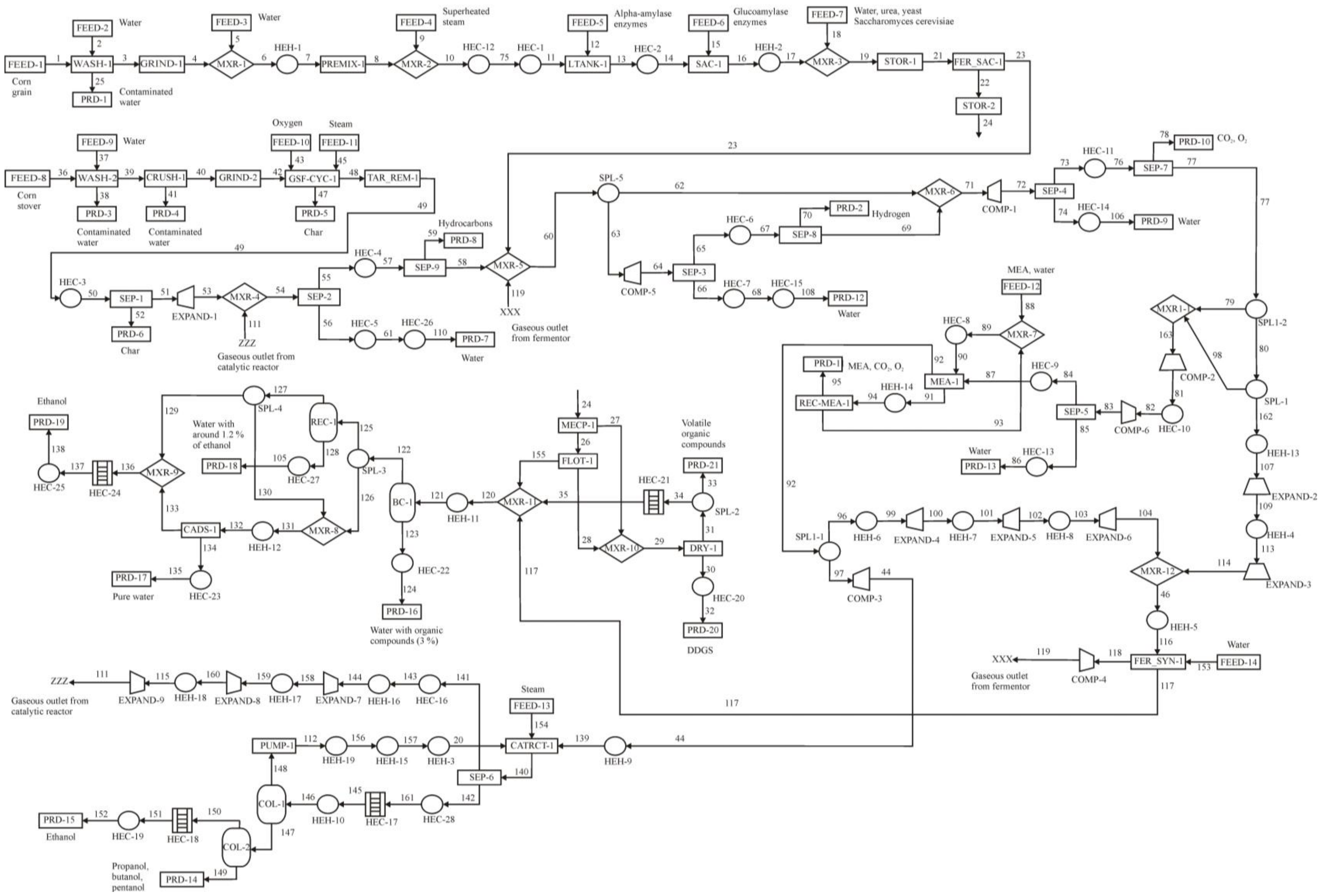


Figure 3-4. Detailed superstructure of the integrated process

Further, energy is then integrated within the process. The dry-grind process requires energy, whilst the generation of energy at the reactors occurs at low temperatures and cannot be reused. On the other hand the thermochemical process (gasification and catalytic synthesis) generates energy. Therefore, the hot streams of the thermo-chemical process are used to provide energy to the, in general, low temperature process streams of the biochemical process.

The prices for raw materials, products and utilities taken for the optimisation are shown in Table 3-1.

Table 3-1. Prices for raw materials, products and utilities used during the process

Raw material	Price ($/t)	Product	Price ($/t)	Utility	Price ($/MWh)
Corn grain	154	Ethanol	786.9	Electricity	60
Corn stover	30	Hydrogen	1,580	Cooling water	4.25
Water	0.061	DDGS	170	Steam	33.7
Oxygen	21				
MEA	1,250				

The main objective of the problem is minimising the costs of both integrated processes. The model by (Duran and Grossmann, 1986), already implemented in MIPSYN, was used for the simultaneous optimisation and HI.

The MINLP problem is decomposed into two subproblems (NLP’s), one per alternative technology for processing corn stover. The integrated biochemical and thermo-biochemical process consists of around 21,500 equations and 22,650 variables, and can be solved in 8.2 s of CPU time, and the integrated biochemical and thermo-chemical process consists of around 23,000 equations and 24,300 variables, and can be solved in approximately 17 s of CPU time. Both NLP’s are performed using CONOPT/GAMS on a personal computer with Intel® Core™2 Quad Q8200 processor with 3.25 GB of RAM.

3.3 Results and Discussion

Integration of raw materials, energy, and process technologies for the production of ethanol from the entire corn plant includes a number of compromise solutions for determining the optimally-integrated process.

The integrated dry-grind process and gasification and syngas fermentation process contains the common technology route for ethanol dehydration, thereby reducing investment cost. The ethanol yield is higher in comparison with the integrated biochemical and thermochemical process (8.6 kg/s vs. 8.02 kg/s). However, the low operating temperature within the fermentor (38 °C) does allow for neither good HI, nor the extraction of energy from exothermic reactor, thereby increasing the need for utilities.

The integrated dry-grind process and gasification and catalytic synthesis process provides a good opportunity for HI, since catalytic reaction takes place at high pressure and temperature, and the reactions are exothermic. Heat can be usefully employed within energy-intensive operations, such as distillations. This process requires separate production lines, which brings increased investment cost. It also provides a lower ethanol yield compared with the integrated biochemical and thermo-biochemical process. On the other hand, with this integrated technology, higher hydrogen yields are obtained (0.33 kg/s vs. 0.29 kg/s), which significantly contributes to the profitability of the process. The advantages and disadvantages of integrated technologies are summarised in Table 3-2.

Table 3-2. Advantages and disadvantages of integrated ethanol production technologies

Integrated technology	Advantages	Disadvantages
DGP and GSF	Common distillation and dehydration – lower investment cost (227 M$) Higher ethanol yield (8.6 kg/s)	Weak HI Lower hydrogen yield (0.29 kg/s)
DGP and GCS	More efficient HI Higher hydrogen yield (0.33 kg/s)	Higher investment cost (251 M$) Lower ethanol yield (8.02 kg/s)

*DGP – dry-grind process, GSF – gasification and further syngas fermentation, GCS – gasification and further catalytic synthesis

The main results of the optimisation are shown in Table 3-3.

Table 3-3. Summary of the integrated base-case processes

Process path	Steam (MW)		Cooling (MW)		Electricity (MW)	Cost* ($/kg)	Ethanol (kt/y)
	no HI	HI	no HI	HI			
DGP and GSF	133	63	128	60	-1.83	0.43	266.7
DGP and GCS	97	17	127	50	0.62	0.41	248.5

*production cost includes depreciation, administration, maintenance, other costs, chemicals, labour, utilities and raw materials

The optimal integrated process, which leads to a minimum production cost, is a combined dry-grind process and gasification and catalytic synthesis due to good HI, despite a lower ethanol production rate.

3.3.1 Effect of the Increased Flowrate of Corn Stover

The flowrate of the corn stover is increased. This can be interpreted as either different lignocellulosic materials can be used as a raw material (by assuming that all lignocellulosic materials have the same composition), or that corn stover is used for ethanol production, whilst corn grain for both, energy and food.

Figure 3-5 shows the effect on the production cost of increasing the corn stover flowrate from the base case. It can be seen that by increasing the flowrate of corn stover the production cost decreases, mainly due to the economy of scale and also due to much lower corn stover prices in comparison with corn grain prices (30 $/t vs. 154 $/t).

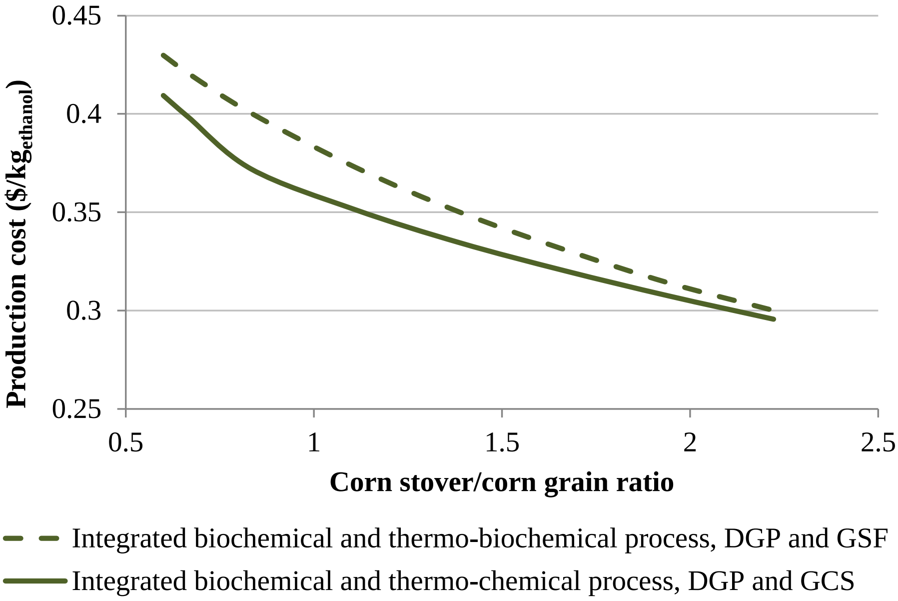


Figure 3-5. Effect of the stover/grain ratio on the production cost (Čuček et al., 2011b)

Production cost of the integrated dry-grind process and gasification and catalytic synthesis are lower compared to alternative integrated process due to good HI. Furthermore, it can be seen that by higher ratios of stover to grain they are approaching production cost of integrated dry-grind process and gasification and syngas fermentation. Within the integrated dry-grind process and gasification and catalytic synthesis, part of the energy could be used for steam production and sold or used somewhere else, which would contribute to better process economy and to lower production cost. However, this option was unconsidered because of potential barriers and to be on the conservative side in terms of production cost. The extreme case, in which only lignocellulosic material is used according to (Martín and Grossmann, 2011a), is the most profitable process for producing ethanol as long as its demand can be met with the harvested lignocellulosic raw material, whilst the use of grain is left for food production.

Figure 3-6 presents the effect of increasing the flowrate of corn stover on energy consumption. From the integrated dry-grind process and gasification and catalytic synthesis process it can be seen from the ratios of stover to grain being equal to one and larger, that heating energy is no longer needed and the cooling requirements start to increase. Under these conditions 43 % of the grain is used for food, and all the remaining grain and stover for ethanol production.

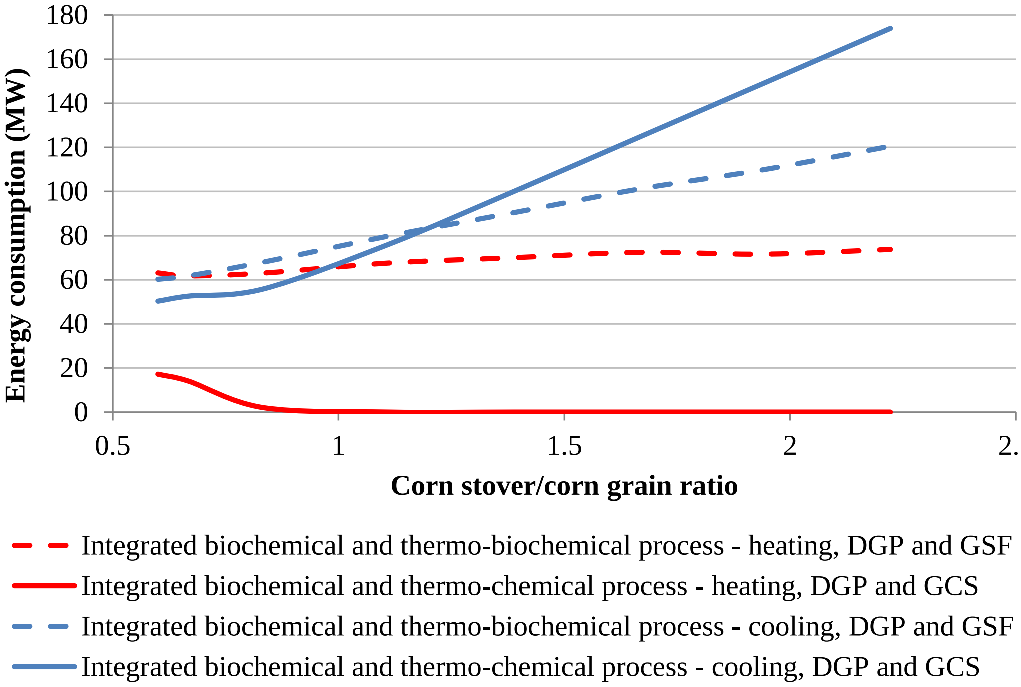


Figure 3-6. Effect of the stover/grain ratio on the energy consumption (Čuček et al., 2011b)

The HI model (Duran and Grossmann, 1986) implemented in MIPSYN is used for simultaneous HI and process integration, which uses the method of pinch candidates. The results clearly indicate that an excess of energy has to be removed from the process for stover/grain ratios larger than around 0.8, however this option is excluded within the synthesis. This leads to larger needs for cooling utilities, as the surplus of energy has to be removed from the process.

In the case of the dry-grind process and gasification and syngas fermentation process, the excess of energy from the gasification and syngas fermentation process is used within the dry-grind process. When increasing the capacity of the gasification and syngas fermentation process, more energy is available for the integration. However, the amount of energy is limited due to the low temperature operations within the reactors and high energy consumption during distillation. Nevertheless, this process requires a lot of energy, resulting in an increase in energy needs.

The ethanol yield from the two integrated production processes reduces by increasing the amount of the corn stover within the process, see Figure 3-7.

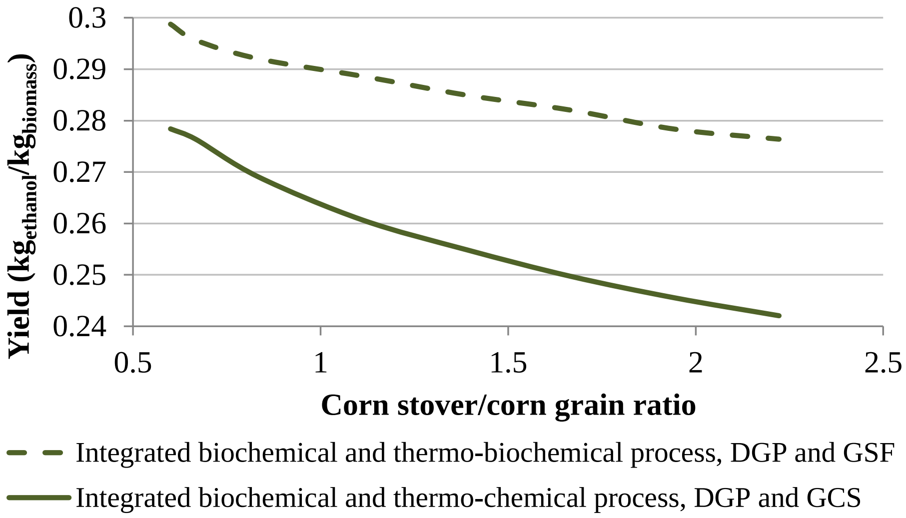


Figure 3-7. Effect of the ratio stover/grain on the ethanol yield (Čuček et al., 2011b)

The ethanol yield from the dry-grind process is higher compared to both conversion paths for processing corn stover. A higher ethanol yield is obtained from the gasification and syngas fermentation process than from the gasification and catalytic synthesis, see also Table 3-3. From Figure 3-7 it can be seen that the ethanol yield decreases faster in the case of the integrated dry-grind process and gasification and catalytic synthesis process.

3.3.2 Sensitivity Analysis

The biomass prices change very rapidly, they depend on the harvest, weather and market conditions, etc. The price of corn grain has fluctuated considerably over the past five years from about 100 $/t in December 2005 to more than 330 $/t in July 2012, and was around 300 $/t in January 2013 (IndexMundi, 2013).

Therefore, a sensitivity analysis is performed to evaluate the effect of the grain and stover prices on the production cost of bioethanol that uses an integrated gasification and catalytic synthesis process for corn stover and dry-grind process for corn grain. The prices of corn grain vary from 154 $/t, to 200, 250, 300, up to 350 $/t. It is also predicted that the corn stover price could most probably be doubled or even tripled. The price of corn stover is increased from 30 $/t to 45, 60, 75, up to 100 $/t.

The results are presented in Figure 3-8 for the effect of the corn grain price on the production cost, and in Figure 3-9 for the effect of the corn stover price on the production cost of the integrated process.

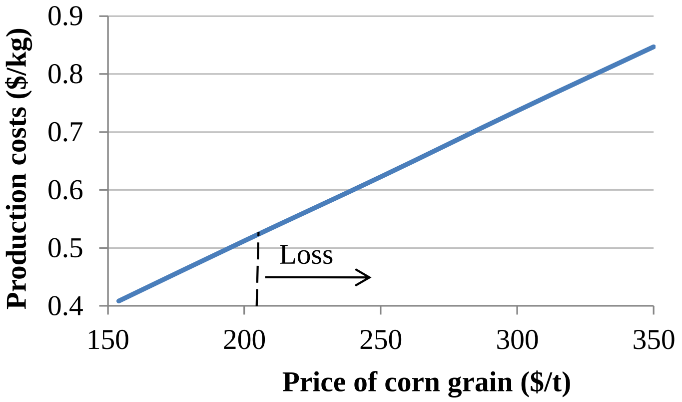


Figure 3-8. Effect of the corn grain price on the production cost of the integrated process (Čuček et al., 2011b)

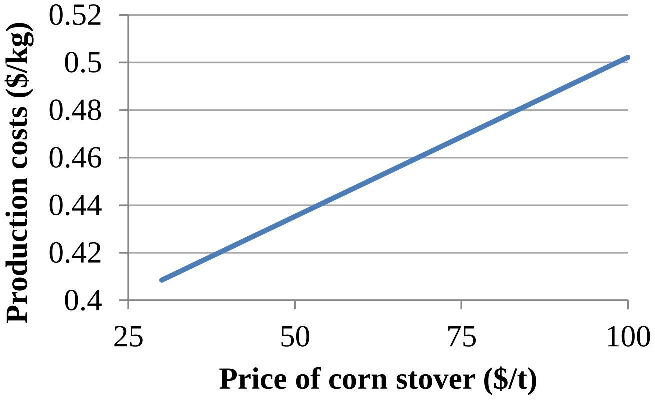


Figure 3-9. Effect of corn stover price on the production cost of the integrated process (Čuček et al., 2011b)

From Figure 3-8 and Figure 3-9 it can be seen that an increase in the corn grain price leads to an increase in the ethanol production costs of 0.0224 $/kg per 10 $/t of increase in the raw material, whilst an increase in the corn stover price adds an ethanol production cost of 0.0134 $/kg per 10 $/t of increase in the stover cost. However, if the price of grain increases over 200 $/t, see Figure 3-8, the profit turns into a loss (-25 M$/y by the corn grain price of 250 $/t). From this analysis it is evident that corn grain is a key component, which is critical for the profitability of an integrated process. At the higher corn grain prices, it is obvious that it makes more sense to produce food from the grains, rather than using grain for fuel.

4 SYNTHESIS OF A REGIONAL NETWORK FOR THE PRODUCTION OF BIOMASS PRODUCTS

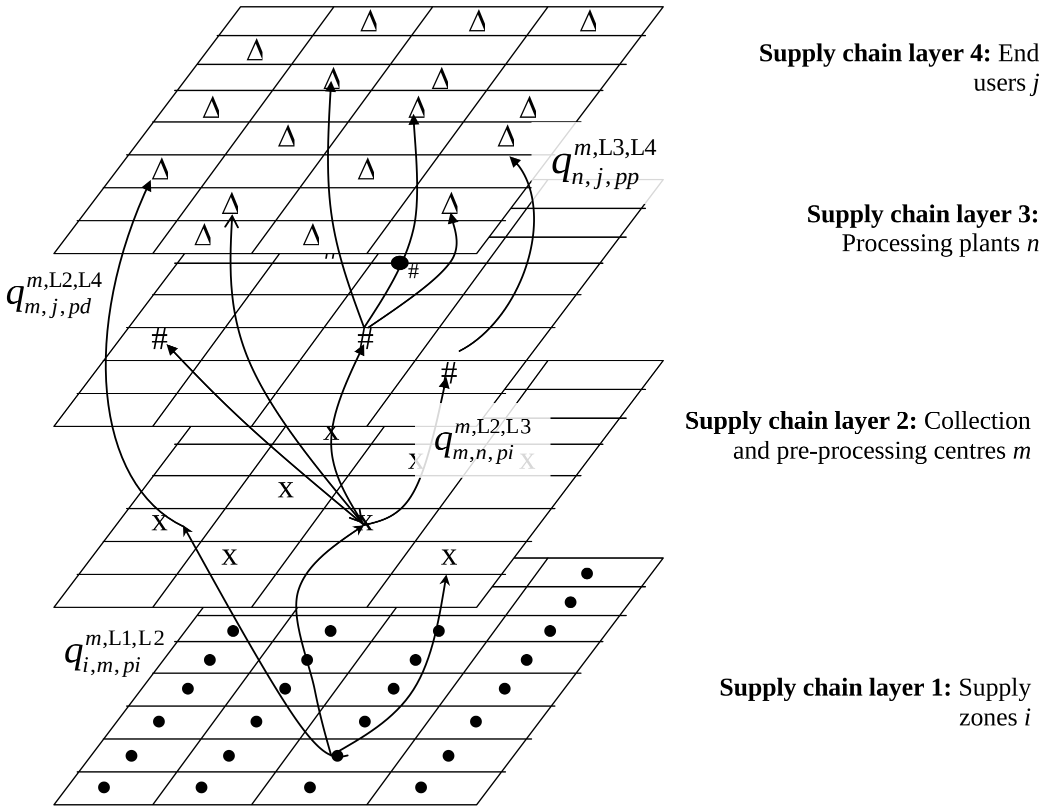
This Chapter is divided into two parts. In the first part it shortly presents the simple synthesis of the regional network for the production of bioproducts (Čuček et al., 2010), and in the second part the upgraded synthesis, the multi-period synthesis of biorefinery's supply networks (Čuček et al., 2013c).

4.1 Synthesis of a Network for the Production of Bioproducts

The aim of this work is to develop a generic (independent from data) synthesis model of a regional renewable energy supply chain based on MP. An integrated MILP model is developed for efficient biomass network optimisation on a regional scale. A four layer supply chain superstructure has been developed, which contains set of potential locations of: i) harvesting sites at supply zones (layer 1 – L1), ii) collection, pre-processing, and storage facilities (layer 2 – L2), iii) conversion technologies (layer 3 – L3), and iv) end-users (layer 4 – L4), and also includes the connection links between these layers. Food-based products can be used either at demand locations, without transforming them into bioproducts, or transformed within processing technologies at L3 into biofuels and other bioproducts. The region is divided into a number of zones for optimising the conversion operation and transportation flows. The model is capable of accounting for different biomass types, optimising the locations, types and capacities of the processing plants and the connecting logistic networks. A four-layer supply chain design is presented in Figure 4-1.

This model, and an illustrative example, are further extended to account for a variety of direct, indirect and total footprints (Čuček et al., 2012e) (see Section 5.1), and reducing the number of direct footprints to a minimum number of representative ones (Čuček et al., 2013a) (see Chapter 6). This model is also extended to a multi-period one accounting for several additional features (see Section 4.2).

The developed mathematical model consists of mass balances, production, and conversion constraints, transportation, operating and capital costs, economic objective function (maximising the profit before tax, *P*), and environmental impact calculation (only CF is evaluated). The demand in the region is defined, and the products exceeding the demand are sold. The MP of the MILP model was performed using GAMS. Equations for evaluating the environmental impact are defined within a more comprehensive context in Section 5.1.



Legend: ● Supply zone x Collection centre # Processing plant

Δ End user $q^{m,La,Lb}_{x,y,p}$ Mass-flow of product *p* from *x* in L*a* to *y* in L*b*

Figure 4-1. Four layer supply chain design (modified from (Lam et al., 2011))

4.1.1 Illustrative Example

The generic optimisation model is tested on the illustrative example of the smaller region (Lam, 2010). The region is divided into 10 zones, each with an area of 100 km^2. The regional plan of the illustrative example is presented in Figure 4-2, where the regional features can be shown.

Several biomass types, technology options, and bioproducts are considered in the synthesis. The utilised biomass types are corn grain, corn stover, wood chips, timber, MSW, and manure. Technologies considered for converting biomass to bioproducts are dry-grind process, AD, MSW incineration, timber sawing, and incineration. The produced bioproducts are electricity, heat, bioethanol, boards, organic fertiliser (digestate), and DDGS. A revenue of the base-case process of 34 M€/y is obtained.

More details regarding this model, an illustrative example and obtained results can be found in (Lam, 2010).

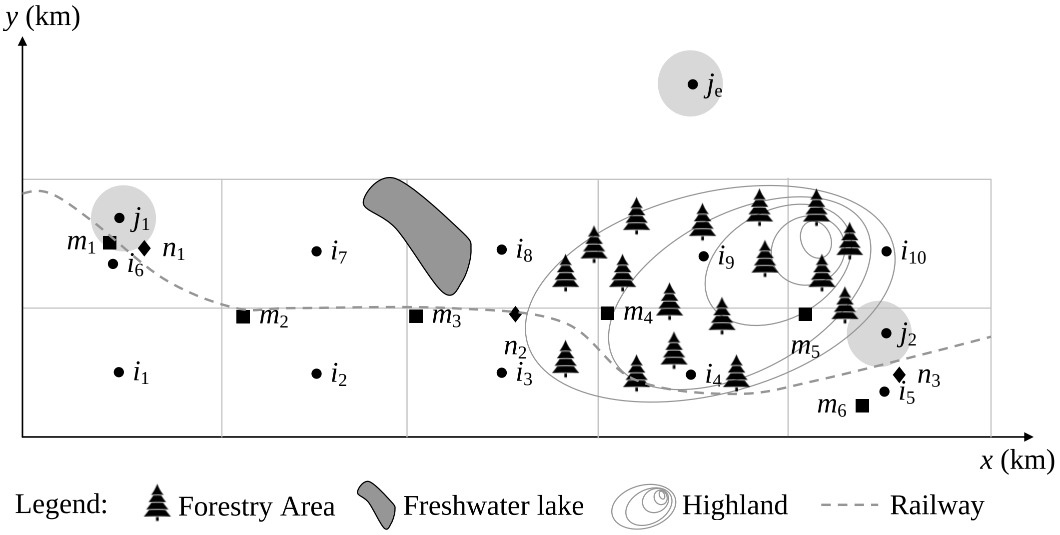


Figure 4-2. Regional plan for the illustrative example (Čuček et al., 2010)

4.2 Multi-Period Synthesis of a Biorefinery's Supply Networks

The generic synthesis model, briefly presented in the previous Section 4.1, is extended to a multi-period model including several additional features, in order to be even more useful for real-world applications, and for decision-making. It accounts for the seasonality and availability of biomass resources, optimal time periods and capacities when facilities are operating, harvesting loss, intermediate storage at L2 and L3, biomass and bioproducts degradation over time related to storage, optimal selection of areas during the year for each year-round biomass resource, and optimal harvesting period(s) for seasonal biomass resources. It includes the possibilities of purchasing additional raw materials, not produced within the region, at L2 and L3. It also enables the produced products from one technology to be recycled and used within other technologies at L2 and L3, which use them as raw materials. Also the excess of energy at different levels can be reused within the same or within another technology at L2 and L3, accounting for heat loss during distribution and the cost of the heat-distribution system. This model also considers the competition between fuels and food production. Multi-period synthesis of a heat-integrated biorefinery's supply network is performed, with maximisation of the economic performance.

The synthesis model employs a four layer structure: i) harvesting sites at supply zones at L1, ii) collection, pre-processing and storage facilities at L2, iii) biorefineries and storage facilities at L3, and iv) end-users at L4, including logistics. The general superstructure of the analysed supply chain network is presented in Figure 4-3, where the differences with a simpler design, as shown in Figure 4-1, can also be seen.

For each specific layer, the following should be specified:

- For each harvesting site:
  - Availability of area within each zone;

  - Availability of each seasonal and year-round resource;
  - Hectare yields per harvesting period of each resource;
  - Unit cost of each resource;
  - Harvesting loss.
- For each potential collection, pre-processing and storage facility:
  - Fixed and variable cost of facility construction;
  - Unit cost of biomass and waste pre-processing, and storage;
  - Conversion factors of the intermediate product in regard to the raw material;
  - Conversion factors of additionally-purchased or recycled products in regard to the key intermediate product;
  - Unit cost of additionally-purchased raw material;
  - Intermediate and by-products' yield;
  - Degradation percentage of intermediate product during storage;
  - Cost and capacities of the different reference pre-processing technologies;
  - Operating cost of each pre-processing technology;
  - Minimal and maximal capacity of collection, pre-processing, and storage facility;
  - Water consumption, and energy consumption and production within different reference pre-processing technologies.

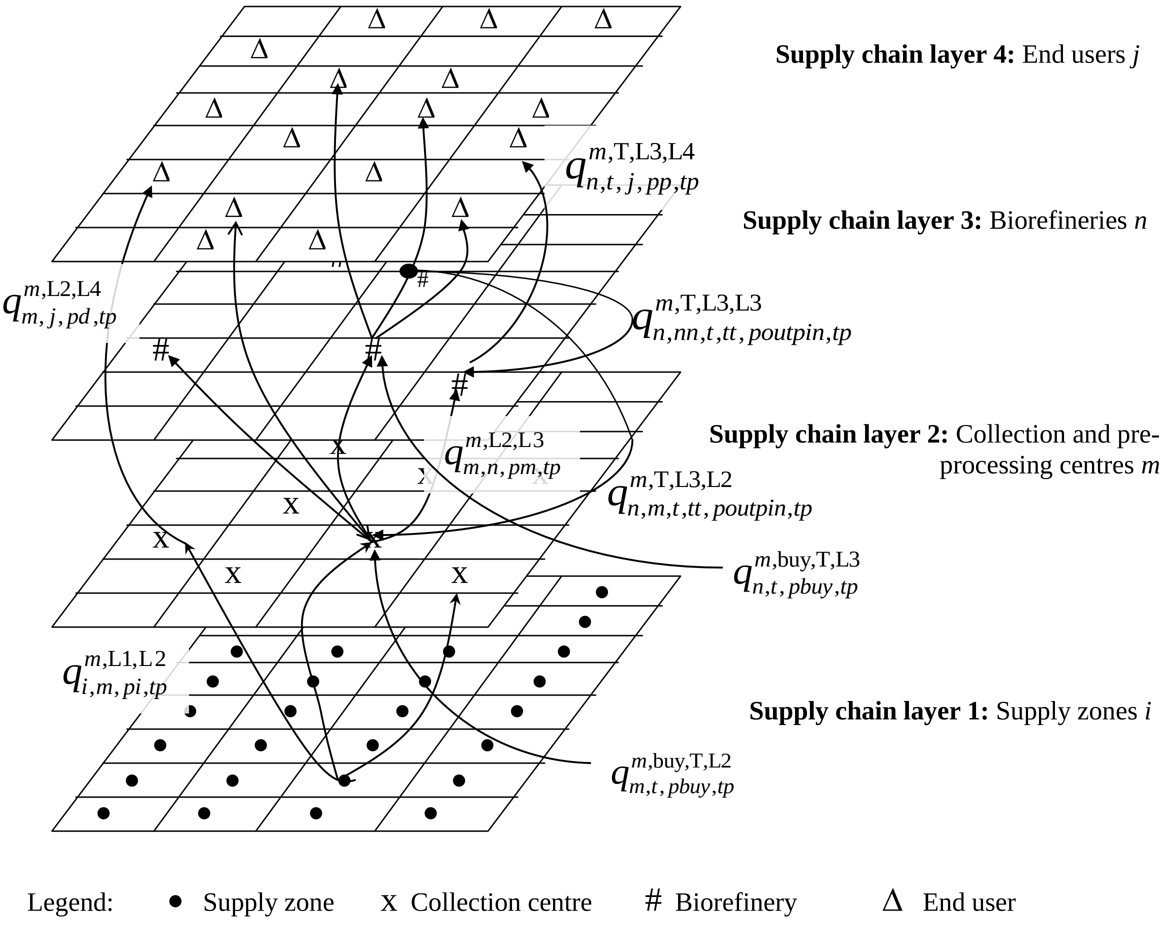


Figure 4-3. Extended four-layer supply chain design (modified from (Lam et al., 2011))

- For each potential biorefinery process:
  - Conversion factors of the produced product in regard to the intermediate product;
  - Conversion factors of additionally-purchased or recycled products in regard to the key produced product;
  - Unit cost of additionally-purchased raw material;
  - Biofuels and by-products yield;
  - Cost and capacities of the different reference processing technologies;
  - Operating cost of each specific biofuel technology route;
  - Water consumption, and energy consumption and production of different reference processing technologies;
  - Unit cost of products' storage;
  - Degradation of biofuel and by-product during potential storage;
  - Minimal and maximal capacity of processing plant and storage facility.
- For each potential demand location:
  - Food, biofuel and by-product demand in each time period;
  - Unit price of each direct and produced product;
- For each transportation and distribution link:
  - Transportation capacity (in both volume and weight);
  - Available transportation modes;
  - Unit transportation and distribution costs of each mode;
  - Distances between potential locations;
  - Loss of material due to distributing it over a distance.

The advantages of this work are: i) in the systematic analysis of using optimal raw materials, production processes, and products, and ii) in developing a generic mathematical model (independent from data), that could be used for any biomass supply chain network, within any region, state or country.

4.2.1 Mathematical Model

The model is formulated as an MILP. The model consists of mass balances, production, and conversion constraints, cost functions, and economic objective function. It follows the four-layer (L1 – L4) nature of the network's superstructure (see Figure 4-3), starting from the harvesting and supply (L1) layer, collection and pre-processing (L2), main processing (L3), up to the use (L4) layer. It includes intermediate storage at L2 and L3, and the transportation links between and within the layers.

The following sets and subsets are defined within the model (Equations (4.1) – (4.64)):

i) Set I for supply zones within L1 with elements $i \in I$.

ii) Set J for demand locations within L4 with elements $j \in J$.

iii) Set M for collection and intermediate process centres within L2 with elements $m \in M$.

iv) Set N for biorefineries within L3 with elements $n \in N$.

v) Set NI for intervals with elements $ni \in NI$.

vi) Set P for the products with elements $p \in P$.

vii) Set T for process technology options with elements $t \in T$.

viii) Set TP for time periods with elements $tp \in TP$.

ix) Set KP for key product ($KP \subseteq (PM \cup PP)$) with elements $kp \in KP$.

x) Set $PADD$ for additional resources needed for conversion besides main resources $(PADD \subseteq P = PBUY \cup POUTPIN)$ with elements $padd \in PADD$.

xi) Set $PBUY$ for purchased raw materials $(PBUY \subseteq P)$ with elements $pbuy \in PBUY$.

xii) Set PD for directly used products $(PD \subseteq P)$ with elements $pd \in PD$.

xiii) Set PI for intermediate products $(PI \subseteq P)$ with elements $pi \in PI$.

xiv) Set $PICON$ for year-round resources $(PICON \subseteq P)$ with elements $picon \in PICON$.

xv) Set $PIPM \subseteq PI \times PM$ for pairs of resource and pre-treated product (if a pre-treated product is from a given resource) with elements $(pi, pm) \in PIPM$.

xvi) Set $PISE$ for seasonal biomass resources $(PISE \subseteq P)$ with elements $pise \in PISE$.

xvii) Set $PIT \subseteq PI \times T$ for pairs of intermediate product and applicable process technology for it with elements $(pi,t) \in PIT$.

xviii) Set PM for stored and pre-treated products (intermediate products) coming from the layer L2 $(PM \subseteq P)$ with elements $pm \in PM$.

xix) Set $PMPP \subseteq PM \times PP$ of intermediate and produced products (if a produced product is from a given intermediate product) with elements $(pm, pp) \in PMPP$.

xx) Set $PMT \subseteq PM \times T$ of pairs of product *pm*, and the applicable process technology for it with elements $(pm,t) \in PMT$.

xxi) Set $POUTPIN$ for recycled produced products from one technology to another $(POUTPIN \subseteq P)$ with elements $poutpin \in POUTPIN$.

xxii) Set PP for produced products coming from the layer L3 $(PP \subseteq P)$ with elements $pp \in PP$.

xxiii) Set $PPT \subseteq PP \times T$ of pairs of product *pp*, and its applicable process technology with elements $(pp,t) \in PPT$.

xxiv) Set $T_2 \subseteq T$ for technology options at pre-processing facilities with elements $t \in T_2$.

xxv) Set $T_3 \subseteq T$ for technology options at processing plants with elements $t \in T_3$.

xxvi) Set $TKP \subseteq T \times KP$ for pairs of technology and produced key product (if a key product is produced from a given technology) with elements $(t, kp) \in TKP$.

xxvii) Set $TTPADD \subseteq PADD \times T$ for pairs of technology and additional resource needed (if an additional resource is needed for a given technology) with elements $(padd, tt) \in TTPADD.$

xxviii) Set $TTTNM \subseteq N \times M \times T \times TT \times POUTPIN$ for quintuples of plant location *n*, storage and pre-processing location *m*, technology *t* at L3, technology *tt* at L2, and recycled produced product *poutpin* (if product is recycled from technology *t* at L3 to technology *tt* at L2) with elements $(n, m, t, tt, poutpin) \in TTTNM$.

xxix) Set $TTTP \subseteq N \times NN \times T \times TT \times POUTPIN$ for quintuples of plant locations *n* and *nn*, technology *t* at location *n*, technology *tt* at *nn*, and recycled produced product *poutpin* (if product is recycled from technology *t* at *n* to technology *tt* at *nn*) with elements $(n, nn, t, tt, poutpin) \in TTTP.$

xxx) Set *UTILITY* for process utility $(UTILITY \subseteq P)$ with elements $utility \in UTILITY$.

4.2.1.1 Mass Balances, Production and Conversion Constraints

The area available for growing biomass resources $(pi \in PI)$ in zone $(i \in I)$ to be used for the purpose of energy and bioproducts production $(A_{i,pi})$ should be less than or equal to the fraction of area intended for energy in that zone (x_i) multiplied by the whole area (A_i^{UP}).

$$\sum_{pi \in PI} A_{i,pi} \leq x_i \cdot A_i^{\mathrm{UP}} \qquad \forall i \in I \tag{4.1}$$

The sum of areas for seasonal biomass resources $(pise \in PISE \subseteq PI)$ over all time periods $(tp \in TP)$ should be equal to the whole area intended for this biomass type $(A_{i,pise})$:

$$\sum_{tp \in TP} A_{i,pise,tp} = A_{i,pise} \qquad \forall (i \in I, pise \in PISE) \tag{4.2}$$

For the year-round resources $(picon \in PICON \subseteq PI)$ within each time period $(A_{i,picon,tp})$ there are two options, either the area should be equal to the whole area intended for this biomass type $(A_{i,picon})$ (Equation (4.3)) or less than or equal to the whole area intended for this biomass type (Equation (4.4)). The first case means that the area is constant throughout the year, whilst the second case means that the selected area for year-round raw materials could be different for each month. It should be noted, that during both cases seasonal raw materials could be harvested over optimal time period(s).

$$A_{i,picon,tp} = A_{i,picon} \qquad \forall (i \in I, picon \in PICON, tp \in TP) \tag{4.3}$$

$$A_{i,picon,tp} \leq A_{i,picon} \qquad \forall (i \in I, picon \in PICON, tp \in TP) \tag{4.4}$$

The production rate of a particular biomass and waste type $(pi \in PI, PI = PISE \cup PICON)$ at supply zone *i* and time period *tp*, subject to the yield of biomass type *pi* in time period *tp* $(HY_{pi,tp})$, and available area at zone *i* and time period *tp*, is expressed via constraint (4.5):

$$q^{m,\mathrm{L1}}_{i,pi,tp} = HY_{pi,tp} \cdot A_{i,pi,tp} \qquad \forall (pi \in PI, i \in I, tp \in TP) \tag{4.5}$$

Raw material *pi* produced at zone *i* and time period *tp* is transported to storage and pre-processing centers $(m \in M)$:

$$q^{m,\mathrm{L1}}_{i,pi,tp} = \sum_{m \in M} q^{m,\mathrm{L1,L2}}_{i,m,pi,tp} \qquad \forall (pi \in PI, i \in I, tp \in TP) \tag{4.6}$$

The available area for crop residues at zone *i* and time period *tp*, should be less than or equal to the area available for grains at zone *i* and time period *tp*:

$$A_{i,\mathrm{grain},tp} \geq A_{i,\mathrm{crop\ residue},tp} \qquad \forall (i \in I, tp \in TP) \tag{4.7}$$

Raw material type *pi* deducted by harvesting loss L_{pi}, is sent to the selected preprocessing technology or storage *t*:

$$\sum_{i \in I} q^{m,\mathrm{L1,L2}}_{i,m,pi,tp} \cdot (1 - L_{pi}) = \sum_{(pi,t) \in PIT \wedge t \in T_2} q^{m,\mathrm{T,L2}}_{m,pi,t,tp} \qquad \forall (m \in M, pi \in PI, tp \in TP) \tag{4.8}$$

Raw material type *pi* is converted into the intermediate product $pm \in PM$ using the corresponding conversion factor $(f^{\mathrm{conv,T,L2}}_{pi,pm,t})$. Process conversion is handled as the amount of the intermediate product flowrate compared to the inlet flowrate of the biomass raw material to the pre-processing and storage facilities.

$$q^{m,\mathrm{T,L2}}_{m,pi,t,tp} \cdot f^{\mathrm{conv,T,L2}}_{pi,pm,t} = q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp} \qquad \forall (m \in M, tp \in TP, (pi,t) \in PIT, (pi,pm) \in PIPM) \tag{4.9}$$

Equations (4.10) – (4.12) are used to determine the selection or rejection the preprocessing technologies. Preprocessing facilities have to operate within minimal and maximal capacities. Equation (4.10) represents the minimum capacity of storage and preprocessing facility during the facility life-time $(q^{m,\mathrm{T,LO}}_{t})$, Equation (4.11) maximum capacity of facility at each time period *tp* $(q^{m,\mathrm{T,UP}}_{t,tp})$, and Equation (4.12) maximum capacity of the facility during its life-time $(q^{m,\mathrm{T,UP}}_{t})$.

$$\sum_{(pi,t) \in PIT} \sum_{(pi,pm) \in PIPM} \sum_{(t,pm) \in TKP} \sum_{tp \in TP} q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp} \geq q^{m,\mathrm{T,LO}}_{t} \cdot y^{\mathrm{T,L2}}_{m,t} \qquad \forall (m \in M, t \in T_2) \tag{4.10}$$

$$\sum_{(pi,t) \in PIT} \sum_{(pi,pm) \in PIPM} \sum_{(t,pm) \in TKP} q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp} \leq q^{m,\mathrm{T,UP}}_{t,tp} \cdot y^{\mathrm{T,L2}}_{m,t,tp} \qquad \forall (m \in M, t \in T_2, tp \in TP) \tag{4.11}$$

$$\sum_{(pi,t)\in PIT}\ \sum_{(pi,pm)\in PIPM}\ \sum_{(t,pm)\in TKP}\ \sum_{tp\in TP} q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp} \le q^{m,\mathrm{T,UP}}_{t}\cdot y^{\mathrm{T,L2}}_{m,t} \qquad \forall(m\in M, t\in T_2) \tag{4.12}$$

Additional resources $(padd \in PADD = PBUY \cup POUTPIN)$ needed for the conversion of biomass and waste type *pi* to intermediate products *pm* are either purchased ($q^{m,\mathrm{buy,T,L2}}_{m,tt,pbuy,tp}$) or recycled from other production technologies $(q^{m,\mathrm{net,T,L3,L2}}_{n,m,t,tt,poutpin,tp})$ and are defined per key intermediate product $(kp \in KP)$:

$$\begin{aligned}\sum_{(pi,tt)\in PIT}\ \sum_{(pi,kp)\in PIPM} q^{m,\mathrm{T,L2}}_{m,pi,pm,tt,tp}\cdot f^{\mathrm{conv,add,T}}_{tt,padd,kp} = \sum_{pbuy\in PADD} q^{m,\mathrm{buy,T,L2}}_{m,tt,pbuy,tp} + \\ \sum_{(n,m,t,tt,poutpin)\in TTTNM} q^{m,\mathrm{net,T,L3,L2}}_{n,m,t,tt,poutpin,tp} \\ \forall(m\in M, (padd,tt)\in TTPADD \wedge tt\in T_2, tp\in TP)\end{aligned} \tag{4.13}$$

Since the model is multi-periodic and accounts for variability of supply and demand, it has to include intermediate storage at L2 and L3. The quantity of intermediate product at L2 at time period *tp* $(m^{\mathrm{L2}}_{m,pm,tp})$ is sum of quantity of intermediate products from previous time period $(m^{\mathrm{L2}}_{m,pm,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))})$ plus inlet to intermediate storage at time period *tp* $(q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp})$ minus outflows of intermediate products to processing plants $(q^{m,\mathrm{L2,L3}}_{m,n,pm,tp})$, outflows of direct products to consumers $(q^{m,\mathrm{L2,L4}}_{m,j,pd,tp})$, and deterioration of raw material $(\frac{(m^{\mathrm{L2}}_{m,pm,tp} + m^{\mathrm{L2}}_{m,pm,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))})}{2}\cdot Det_{pm,tp})$. The amount of the deteriorated intermediate product is taken as the average quantity of the stored products from two time periods. The storage capacity at L2 is defined with Equation (4.14).

$$\begin{aligned} m^{\mathrm{L2}}_{m,pm,tp} = m^{\mathrm{L2}}_{m,pm,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))} + \sum_{(pi,t)\in PIT}\ \sum_{(pi,pm)\in PIPM} q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp} - \sum_{n\in N} q^{m,\mathrm{L2,L3}}_{m,n,pm,tp} \\ -\sum_{j\in J}\ \sum_{pd\in PM} q^{m,\mathrm{L2,L4}}_{m,j,pd,tp} - \frac{(m^{\mathrm{L2}}_{m,pm,tp} + m^{\mathrm{L2}}_{m,pm,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))})}{2}\cdot Det_{pm,tp} \\ \forall(m\in M, pm\in PM, tp\in TP)\end{aligned} \tag{4.14}$$

Constraints (4.15) and (4.16) are used to determine the selection or rejection of the recycle from production technology *t* at process plant *n* to technology *tt* at storage and pre-processing facility *m* $(q^{m,\mathrm{T,L3,L2}}_{n,m,t,tt,poutpin,tp})$. The recycles have to be within the minimal $(q^{m,\mathrm{T,LO}}_{tt,tp})$ and maximal $(q^{m,\mathrm{T,UP}}_{tt,tp})$ bounds:

$$\begin{aligned}\sum_{tp\in TP} q^{m,\mathrm{T,L3,L2}}_{n,m,t,tt,poutpin,tp} \ge \sum_{tp\in TP} q^{m,\mathrm{T,LO}}_{tt,tp}\cdot y^{\mathrm{L3,L2}}_{n,m,poutpin} \\ \forall((n,m,t,tt,poutpin)\in TTTNM)\wedge poutpin\in UTILITY)\end{aligned} \tag{4.15}$$

$$\sum_{tp \in TP} q_{n,m,t,tt,poutpin,tp}^{m,\mathrm{T,L3,L2}} \le \sum_{tp \in TP} q_{tt,tp}^{m,\mathrm{T,UP}} \cdot y_{n,m,poutpin}^{\mathrm{L3,L2}}$$
$$\forall ((n,m,t,tt,poutpin) \in TTTNM) \wedge poutpin \in UTILITY) \qquad (4.16)$$

The intermediate product *pm* from L2 is sent to the selected plant *n* with technology *t* at L3:

$$\sum_{m \in M} q_{m,n,pm,tp}^{m,\mathrm{L2,L3}} = \sum_{(pm,t) \in PMT \wedge t \in T_3} q_{n,pm,t,tp}^{m,\mathrm{T,L3}} \qquad \forall (n \in N, pm \in PM, tp \in TP) \qquad (4.17)$$

The intermediate product *pm* is converted into the produced product *pp* using the corresponding conversion factor $(f_{pm,pp,t}^{\mathrm{conv,T,L3}})$. Process conversion is handled as the amount of the product flowrate compared to the key inflow of the pre-treated raw material.

$$q_{n,pm,t,tp}^{m,\mathrm{T,L3}} \cdot f_{pm,pp,t}^{\mathrm{conv,T,L3}} = q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}}$$
$$\forall (n \in N, (pm,t) \in PMT, (pm,pp) \in PMPP, tp \in TP) \qquad (4.18)$$

Equations (4.19) – (4.21) are used to determine the selection or rejection the process technologies *t* at process plants *n*. Process plants have to operate within minimal and maximal capacities. Equation (4.19) represents the minimum plant's capacity during the entire year $(q_t^{m,\mathrm{T,LO}})$, Equation (4.20) maximum plant's capacity over each time period $(q_{t,tp}^{m,\mathrm{T,UP}})$, and Equation (4.21) maximum plant's capacity during its life-time $(q_t^{m,\mathrm{T,UP}})$.

$$\sum_{(pm,t) \in PMT} \sum_{(pm,pp) \in PMPP} \sum_{(t,pp) \in TKP} \sum_{tp \in TP} q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}} \ge q_t^{m,\mathrm{T,LO}} \cdot y_{n,t}^{\mathrm{T,L3}} \qquad \forall (n \in N, t \in T_3) \qquad (4.19)$$

$$\sum_{(pm,t) \in PMT} \sum_{(pm,pp) \in PMPP} \sum_{(t,pp) \in TKP} q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}} \ge q_{t,tp}^{m,\mathrm{T,LO}} \cdot y_{n,t,tp}^{\mathrm{T,L3}} \qquad \forall (n \in N, t \in T_3, tp \in TP) \qquad (4.20)$$

$$\sum_{(pm,t) \in PMT} \sum_{(pm,pp) \in PMPP} \sum_{(t,pp) \in TKP} \sum_{tp \in TP} q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}} \ge q_t^{m,\mathrm{T,LO}} \cdot y_{n,t}^{\mathrm{T,L3}} \qquad \forall (n \in N, t \in T_3) \qquad (4.21)$$

The intermediate storage at L3 is defined with Equation (4.22). The quantity of produced product *pp* at L3 at time period *tp* $(m_{n,t,pp,tp}^{\mathrm{L3}})$ is the sum of the quantity of products from the previous time period $(m_{n,t,pp,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))}^{\mathrm{L3}})$ plus the inlet to intermediate storage at time period *tp* $(q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}})$, minus outflows of the produced products to consumers $(q_{n,t,j,pp,tp}^{m,\mathrm{T,L3,L4}})$, minus the outflow of recycled products either to technology *tt* at location *nn* $(q_{n,nn,t,tt,poutpin,tp}^{m,\mathrm{T,L3,L3}})$, or to technology *tt* at location *m* $(q_{n,m,t,tt,poutpin,tp}^{m,\mathrm{T,L3,L2}})$, and minus the deterioration of produced product over time $\frac{(m_{n,t,pp,tp}^{\mathrm{L3}} + m_{n,t,pp,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))}^{\mathrm{L3}})}{2} \cdot Det_{pp,tp}$. The amount of the deteriorated product is taken as the average quantity of the stored products from two time periods. It should be noted that technologies *t* and *tt* can be the same or different technologies, as well as plants *n* and *nn* can be plants at the same or at different locations.

$$\begin{aligned}
\sum_{pp\notin UTILITY} m^{\mathrm{L3}}_{n,t,pp,tp} = {} & \sum_{pp\notin UTILITY} m^{\mathrm{L3}}_{n,t,pp,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))} + \sum_{(pm,t)\in PMT}\ \sum_{(pm,pp)\in PMPP} q^{m,\mathrm{T,L3}}_{n,pm,pp,t,tp} \\
& -\sum_{j\in J}\ \sum_{(pp,t)\in PPT} q^{m,\mathrm{T,L3,L4}}_{n,t,j,pp,tp} - \sum_{(n,nn,t,tt,poutpin)\in TTTP} q^{m,\mathrm{T,L3,L3}}_{n,nn,t,tt,poutpin,tp} \\
& - \sum_{(n,m,t,tt,poutpin)\in TTTNM} q^{m,\mathrm{T,L3,L2}}_{n,m,t,tt,poutpin,tp} \\
& - \frac{(m^{\mathrm{L3}}_{n,t,pp,tp} + m^{\mathrm{L3}}_{n,t,pp,((tp-1)\wedge(tp\neq 1))\vee((\max(tp)\wedge(tp=1))})}{2}\cdot Det_{pp,tp} \\
& \forall (n\in N, t\in T, pp\in PP, tp\in TP)
\end{aligned} \tag{4.22}$$

The loss of materials and energy due to transporting and distributing them over the distance is taken into account in Equation (4.23). Net flowrate of recycled material at the preprocessing facility m $(q^{m,\mathrm{net,T,L3,L2}}_{n,m,t,tt,poutpin,tp})$ is the flowrate of that material from processing plant n $(q^{m,\mathrm{T,L3,L2}}_{n,m,t,tt,poutpin,tp})$ with deducted loss. The loss is computed as $(1-L^{\mathrm{tr}}_{poutpin})^{D^{\mathrm{L2,L3}}_{m,n}}$, where $D^{\mathrm{L2,L3}}_{m,n}$ represents the distance between locations of pre-processing facility m at L2, and processing plant n at L3.

$$\begin{aligned}
& q^{m,\mathrm{T,L3,L2}}_{n,m,t,tt,poutpin,tp}\cdot(1-L^{\mathrm{tr}}_{poutpin})^{D^{\mathrm{L2,L3}}_{m,n}} = q^{m,\mathrm{net,T,L3,L2}}_{n,m,t,tt,poutpin,tp} \\
& \qquad \forall((n,m,t,tt,poutpin)\in TTTNM, tp\in TP)
\end{aligned} \tag{4.23}$$

Constraints (4.24) and (4.25) are used to determine the selection or rejection of the utility flows from technology t at plant n to demand location j. The utility flows should be within the lower $(q^{m,\mathrm{T,LO}}_{t,tp})$ and upper $(q^{m,\mathrm{T,UP}}_{t,tp})$ bounds:

$$\sum_{tp\in TP} q^{m,\mathrm{T,L3,L4}}_{n,t,j,pp,tp} \geq \sum_{tp\in TP} q^{m,\mathrm{T,LO}}_{t,tp}\cdot y^{\mathrm{L3,L4}}_{n,j,pp} \qquad \forall(n\in N, j\in J, (pp,t)\in PPT, pp\in UTILITY) \tag{4.24}$$

$$\sum_{tp\in TP} q^{m,\mathrm{T,L3,L4}}_{n,t,j,pp,tp} \leq \sum_{tp\in TP} q^{m,\mathrm{T,UP}}_{t,tp}\cdot y^{\mathrm{L3,L4}}_{n,j,pp} \qquad \forall(n\in N, j\in J, (pp,t)\in PPT, pp\in UTILITY) \tag{4.25}$$

Constraints (4.26) and (4.27) are used to determine the selection or rejection of the utility flows from technology t at plant n to technology tt at plant location nn. The utility flows should be within the lower $(q^{m,\mathrm{T,LO}}_{t,tp})$ and upper $(q^{m,\mathrm{T,UP}}_{t,tp})$ bounds. Note again that technologies t and tt can be the same $(t = tt)$ or different technologies $(t \neq tt)$, and plants n and nn can be plants at the same $(n = nn)$ or at different locations $(n \neq nn)$.

$$\begin{aligned}
& \sum_{tp\in TP} q^{m,\mathrm{T,L3,L3}}_{n,nn,t,tt,poutpin,tp} \geq \sum_{tp\in TP} q^{m,\mathrm{T,LO}}_{t,tp}\cdot y^{\mathrm{L3,L3}}_{n,nn,poutpin} \\
& \qquad \forall((n,nn,t,tt,poutpin)\in TTTP, poutpin\in UTILITY)
\end{aligned} \tag{4.26}$$

$$\begin{aligned}
& \sum_{tp\in TP} q^{m,\mathrm{T,L3,L3}}_{n,nn,t,tt,poutpin,tp} \leq \sum_{tp\in TP} q^{m,\mathrm{T,UP}}_{t,tp}\cdot y^{\mathrm{L3,L3}}_{n,nn,poutpin} \\
& \qquad \forall((n,nn,t,tt,poutpin)\in TTTP, poutpin\in UTILITY)
\end{aligned} \tag{4.27}$$

Net flowrate of recycled material at technology *tt* and processing plant *nn* $(q^{m,\text{net},\text{T},\text{L3},\text{L3}}_{n,nn,t,tt,poutpin,tp})$ is the flowrate of that material from technology *t* and processing plant *n* $(q^{m,\text{T},\text{L3},\text{L3}}_{n,nn,t,tt,poutpin,tp})$ deducing the losses. The loss is computed as $(1-L^{\text{tr}}_{poutpin})^{D^{\text{L3,L3}}_{n,nn}}$, where $D^{\text{L3,L3}}_{n,nn}$ represents the distance between the locations of process plant *n* and plant *nn* at L3. The loss of recycled materials and energy due to transporting and distributing them over the distance is taken into account in Equation (4.28).

$$q^{m,\text{T},\text{L3},\text{L3}}_{n,nn,t,tt,poutpin,tp} \cdot (1-L^{\text{tr}}_{poutpin})^{D^{\text{L3,L3}}_{n,nn}} = q^{m,\text{net},\text{T},\text{L3},\text{L3}}_{n,nn,t,tt,poutpin,tp} \qquad \forall((n,nn,t,tt,poutpin)\in TTTP, tp\in TP) \tag{4.28}$$

Additional resources $(padd \in PADD)$ needed for conversion of intermediate product type *pm* to processed products *pp* are either purchased $(q^{m,\text{buy},\text{T},\text{L3}}_{nn,tt,pbuy,tp})$ or recycled from other production technologies $(q^{m,\text{net},\text{T},\text{L3},\text{L3}}_{n,nn,t,tt,poutpin,tp})$ and are again defined per key product *kp*:

$$\begin{aligned}\sum_{(pm,tt)\in PMT}\ \sum_{(pm,kp)\in PMPP} q^{m,\text{T},\text{L3}}_{nn,pm,pp,tt,tp} \cdot f^{\text{conv,add,T}}_{tt,padd,kp} = \sum_{pbuy\in PADD} q^{m,\text{T},\text{buy},\text{L3}}_{nn,tt,pbuy,tp} + \\ \sum_{(n,nn,t,tt,poutpin)\in TTTP} q^{m,\text{net},\text{T},\text{L3},\text{L3}}_{n,nn,t,tt,poutpin,tp} \\ \forall(nn\in N,(padd,tt)\in TTPADD \wedge tt\in T_3, tp\in TP)\end{aligned} \tag{4.29}$$

Net flowrate of produced product at demand location *j* is the flowrate of that material from technology *t* and processing plant *n* $(q^{m,\text{T},\text{L3},\text{L4}}_{n,t,j,pp,tp})$ with deducted loss related to distribution. The loss related to distribution is computed as $(1-L^{\text{tr}}_{pp})^{D^{\text{L3,L4}}_{n,j}}$, where $D^{\text{L3,L4}}_{n,j}$ represents the distance between locations of process plant *n* at L3 and location of demand *j* at L4. The loss of produced materials and energy due to transporting and distributing them over the distance is taken into account in Equation (4.30).

$$q^{m,\text{T},\text{L3},\text{L4}}_{n,t,j,pp,tp} \cdot (1-L^{\text{tr}}_{pp})^{D^{\text{L3,L4}}_{n,j}} = q^{m,\text{net},\text{T},\text{L3},\text{L4}}_{n,t,j,pp,tp} \qquad \forall(n\in N,(pp,t)\in PPT, j\in J, tp\in TP) \tag{4.30}$$

4.2.1.2 Transportation Cost

The transportation costs are composed of fixed (cost of loading and unloading) and distance variable cost (mostly fuel costs, labour costs and equipment cost). The transportation costs are composed of transportation cost for:

i) biomass resources *pi* from zones *i* at L1 to pre-processing and storage facilities *m* at L2:

$$c_{pi}^{\mathrm{tr,L1,L2}} = \sum_{i\in I}\sum_{m\in M}\sum_{tp\in TP}(c_{pi}^{\mathrm{tr,fix,L1,L2}} \cdot q_{i,m,pi,tp}^{m,\mathrm{L1,L2}} + D_{i,m}^{\mathrm{L1,L2}} \cdot c_{pi}^{\mathrm{tr,var,L1,L2}} \cdot q_{i,m,pi,tp}^{m,\mathrm{L1,L2}}) \qquad \forall pi \in PI \tag{4.31}$$

ii) intermediate products *pm*, excluding utilities $(pm \in PM \wedge pm \notin UTILITY)$, from pre-processing and storage facilities *m* at L2 to process plants *n* at L3:

$$c_{pm}^{\mathrm{tr,L2,L3}} = \sum_{m\in M}\sum_{n\in N}\sum_{tp\in TP}(c_{pm}^{\mathrm{tr,fix,L2,L3}} \cdot q_{m,n,pm,tp}^{m,\mathrm{L2,L3}} + D_{m,n}^{\mathrm{L2,L3}} \cdot c_{pm}^{\mathrm{tr,var,L2,L3}} \cdot q_{m,n,pm,tp}^{m,\mathrm{L2,L3}}) \\ \forall (pm \in PM \wedge pm \notin UTILITY) \tag{4.32}$$

iii) direct products *pd*, excluding utilities $(pd \in PD \wedge pd \notin UTILITY)$, from pre-processing and storage facilities *m* at L2 to demand location *j* at L4:

$$c_{pd}^{\mathrm{tr,L2,L4}} = \sum_{m\in M}\sum_{j\in J}\sum_{tp\in TP}(c_{pd}^{\mathrm{tr,fix,L2,L4}} \cdot q_{m,j,pd,tp}^{m,\mathrm{L2,L4}} + D_{m,j}^{\mathrm{L2,L4}} \cdot c_{pd}^{\mathrm{tr,var,L2,L4}} \cdot q_{m,j,pd,tp}^{m,\mathrm{L2,L4}}) \\ \forall (pd \in PD \wedge pd \notin UTILITY) \tag{4.33}$$

iv) produced products *pp*, excluding utilities $(pp \in PP \wedge pp \notin UTILITY)$, from process plants *n* at L3 to demand location *j* at L4:

$$c_{pp}^{\mathrm{tr,L3,L4}} = \sum_{n\in N}\sum_{t\in T}\sum_{j\in J}\sum_{tp\in TP}\sum_{(pp,t)\in PPT}(c_{pp}^{\mathrm{tr,fix,L3,L4}} \cdot q_{n,t,j,pp,tp}^{m,\mathrm{T,L3,L4}} + D_{n,j}^{\mathrm{L3,L4}} \cdot c_{pp}^{\mathrm{tr,var,L3,L4}} \cdot q_{n,t,j,pp,tp}^{m,\mathrm{T,L3,L4}}) \\ \forall (pp \in PP \wedge pp \notin UTILITY) \tag{4.34}$$

v) produced utilities $(pp \in UTILITY)$ from process plants *n* at L3 to demand location *j* at L4:

$$c_{pp}^{\mathrm{tr,L3,L4}} = \sum_{n\in N}\sum_{j\in J}(D_{n,j}^{\mathrm{L3,L4}} \cdot c_{pp}^{\mathrm{tr,var,L3,L4}} \cdot y_{n,j,pp}^{\mathrm{L3,L4}} + \sum_{D_{n,j}^{\mathrm{L3,L4}}=0} c_{pp}^{\mathrm{tr,var,L3,L4}} \cdot y_{n,j,pp}^{\mathrm{L3,L4}}) \\ \forall (pp \in UTILITY) \tag{4.35}$$

vi) produced products that are recycled, excluding utilities $(poutpin \in POUTPIN \wedge poutpin \notin UTILITY)$, from technology *t* at process plant *n* at L3 to technology *tt* at process plant *nn* at L3:

$$c_{poutpin}^{\mathrm{tr,L3,L3}} = \sum_{n\in N}\sum_{t\in T}\sum_{nn\in N}\sum_{tt\in T}\sum_{tp\in TP}(c_{poupin}^{\mathrm{tr,fix,L3,L3}} \cdot q_{n,nn,t,tt,poutpin,tp}^{m,\mathrm{T,L3,L3}} + D_{n,nn}^{\mathrm{L3,L3}} \cdot c_{poutpin}^{\mathrm{tr,var,L3,L3}} \cdot q_{n,nn,t,tt,poutpin,tp}^{m,\mathrm{T,L3,L3}}) \\ \forall (poutpin \in POUTPIN \wedge poutpin \notin UTILITY) \tag{4.36}$$

vii) produced utilities at process plant *n* $(poutpin \in UTILITY)$ that are recycled from process plant *n* at L3 to process plant *nn* at L3:

$$c^{\mathrm{tr,L3,L3}}_{poutpin} = \sum_{n\in N}\sum_{nn\in N}(D^{\mathrm{L3,L3}}_{n,nn}\cdot c^{\mathrm{tr,var,L3,L3}}_{poutpin}\cdot y^{\mathrm{L3,L3}}_{n,nn,poutpin} + \sum_{D^{\mathrm{L3,L3}}_{n,nn}=D^{\mathrm{L3,L3}}_{nn,n}} c^{\mathrm{tr,var,L3,L3}}_{poutpin}\cdot y^{\mathrm{L3,L3}}_{n,nn,poutpin}) \quad \forall(poutpin\in UTILITY) \tag{4.37}$$

viii) produced utilities at process plant *n* $(poutpin\in UTILITY)$ that are recycled from process plant *n* at L3 to pre-treatment and storage facility *m* at L2:

$$c^{\mathrm{tr,L3,L2}}_{poutpin} = \sum_{n\in N}\sum_{m\in M}(D^{\mathrm{L3,L2}}_{n,m}\cdot c^{\mathrm{tr,var,L3,L2}}_{poutpin}\cdot y^{\mathrm{L3,L2}}_{n,m,poutpin} + \sum_{D^{\mathrm{L3,L2}}_{n,m}=0} c^{\mathrm{tr,var,L3,L2}}_{poutpin}\cdot y^{\mathrm{L3,L2}}_{n,m,poutpin}) \quad \forall(poutpin\in UTILITY) \tag{4.38}$$

The total transportation costs (c^{tr}) are described by Equation (4.39):

$$c^{\mathrm{tr}} = \sum_{pi\in PI} c^{\mathrm{tr,L1,L2}}_{pi} + \sum_{pm\in PM} c^{\mathrm{tr,L2,L3}}_{pm} + \sum_{pd\in PD} c^{\mathrm{tr,L2,L4}}_{pd} + \sum_{pp\in PP} c^{\mathrm{tr,L3,L4}}_{pp} + \sum_{poutpin\in POUTPIN} c^{\mathrm{tr,L3,L3}}_{poutpin} + \sum_{poutpin\in POUTPIN} c^{\mathrm{tr,L3,L2}}_{poutpin} \tag{4.39}$$

4.2.1.3 Storage, Pre-Treatment, Operating and Capital Cost

Constraints (4.40) and (4.41) present the maximal storage capacity at L2 $(m^{\mathrm{L2,UP}}_{m,pm})$ and L3 $(m^{\mathrm{L3,UP}}_{n,t,pp})$, which should be greater than or equal to the maximal storage capacity from each time periods *tp* ($m^{\mathrm{L2}}_{m,pm,tp}$ and $m^{\mathrm{L3}}_{n,t,pp,tp}$):

$$m^{\mathrm{L2}}_{m,pm,tp} \le m^{\mathrm{L2,UP}}_{m,pm} \qquad \forall(m\in M, pm\in PM, tp\in TP) \tag{4.40}$$

$$m^{\mathrm{L3}}_{n,t,pp,tp} \le m^{\mathrm{L3,UP}}_{n,t,pp} \qquad \forall(n\in N, t\in T, pp\in PP, tp\in TP) \tag{4.41}$$

The storage cost for intermediate storage at pre-processing and storage facilities *m* at L2, and at process plant locations *n* at L3 are expressed by Equation (4.42):

$$c^{\mathrm{stor}} = \sum_{m\in M}\sum_{pm\in PM} c^{\mathrm{stor}}_{pm}\cdot m^{\mathrm{L2,UP}}_{m,pm} + \sum_{n\in N}\sum_{pp\in PP} c^{\mathrm{stor}}_{pp}\cdot m^{\mathrm{L3,UP}}_{n,t,pp} \tag{4.42}$$

The pre-treatment cost is defined as unit pre-treatment cost $(c^{\mathrm{pretreat}}_{pm})$ multiplied by the intermediate product flowrate $(q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp})$:

$$c^{\mathrm{pretreat,T}}_{pm,t} = c^{\mathrm{pretreat}}_{pm}\cdot \sum_{m\in M}\ \sum_{(pi,t)\in PIT}\ \sum_{(pi,pm)\in PIPM}\ \sum_{tp\in TP} q^{m,\mathrm{T,L2}}_{m,pi,pm,t,tp} \qquad \forall(pm\in PM, t\in T) \tag{4.43}$$

The operating cost for the collection, storage and intermediate pre-processing technologies *t* at pre-processing and storage facilities *m*, which provide collecting, drying, storing, compaction and other treatment, and for the technologies *t* at the process plants *n* is described by Equation (4.44). Operating cost of each technology *t* in time period *tp* are defined as cost of operation of that technology for each key raw material per unit ($c_{pi,t}^{\mathrm{op,T}}$ and $c_{pm,t}^{\mathrm{op,T}}$) multiplied by flowrate of that raw material (*pi*, *pm*) which is converted to key product ($pm \in KP$ and $pp \in KP$) with technology *t* at pre-processing plant *m* or processing plant *n* ($q_{m,pi,pm,t,tp}^{m,\mathrm{T,L2}}$ and $q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}}$), divided by reference capacity of each process technology *t* ($q_t^{m,\mathrm{T},0}$).

$$c_t^{\mathrm{op,T}} = \sum_{tp\in TP}\sum_{m\in M}\sum_{(pi,t)\in PIT}\sum_{(pi,kp)\in PIPM}\frac{c_{pi,t}^{\mathrm{op,T}}}{q_t^{m,\mathrm{T},0}}\cdot q_{m,pi,pm,t,tp}^{m,\mathrm{T,L2}} + \sum_{tp\in TP}\sum_{n\in N}\sum_{(pm,t)\in PMT}\sum_{(pm,kp)\in PMPP}\frac{c_{pm,t}^{\mathrm{op,T}}}{q_t^{m,\mathrm{T},0}}\cdot q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}} \qquad \forall t\in T \tag{4.44}$$

Constraints (4.45) and (4.46) present the maximal capacity of the technology *t* at L2 ($q_{m,pi,pm,t}^{m,\mathrm{T,L2,UP}}$) and L3 ($q_{n,pm,pp,t}^{m,\mathrm{T,L3,UP}}$), which should be greater than or equal to the maximal capacity in each time period *tp* ($q_{m,pi,pm,t,tp}^{m,\mathrm{T,L2}}$ and $q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}}$) multiplied by the number of time periods *tp* ($|TP|$), to be on the annual basis.

$$q_{m,pi,pm,t}^{m,\mathrm{T,L2,UP}} \geq q_{m,pi,pm,t,tp}^{m,\mathrm{T,L2}}\cdot|TP| \qquad \forall(m\in M,(pi,t)\in PIT,(pi,pm)\in PIPM,(t,pm)\in TKP,tp\in TP) \tag{4.45}$$

$$q_{n,pm,pp,t}^{m,\mathrm{T,L3,UP}} \geq q_{n,pm,pp,t,tp}^{m,\mathrm{T,L3}}\cdot|TP| \qquad \forall(n\in N,(pm,t)\in PMT,(pm,kp)\in PMPP,(t,kp)\in TKP,tp\in TP) \tag{4.46}$$

The capital cost of technologies *t* at L2 and L3 is expressed by a piecewise linear approximation (Bergamini et al., 2008) in order to keep the model linear and to obtain (near) global optimal solutions. The lower bound of the capacity (size variable) for technology *t* at L2 ($q_{m,kp,t,ni=1}^{m,\mathrm{T,L2}}$) and L3 ($q_{n,kp,t,ni=1}^{m,\mathrm{T,L3}}$), is calculated using Equation (4.47) and (4.48), where $ni \in NI$ are interval numbers.

$$q_{m,kp,t,ni=1}^{m,\mathrm{T,L2}} = q_t^{m,\mathrm{T,LO}} \qquad \forall(m\in M,(t,kp)\in TKP) \tag{4.47}$$

$$q_{n,kp,t,ni=1}^{m,\mathrm{T,L3}} = q_t^{m,\mathrm{T,LO}} \qquad \forall(n\in N,(t,kp)\in TKP) \tag{4.48}$$

Capacities for technology *t* at L2 ($q_{m,kp,t,ni}^{m,\mathrm{T,L2}}$) and L3 ($q_{n,kp,t,ni}^{m,\mathrm{T,L3}}$), for each interval $ni \in NI, ni > 1$ are calculated using Equations (4.49) and (4.50):

$$q_{m,kp,t,ni}^{m,\mathrm{T,L2}} = q_{m,kp,t,ni=1}^{m,\mathrm{T,L2}} + \frac{q_t^{m,\mathrm{T,UP}} - q_{m,kp,t,ni=1}^{m,\mathrm{T,L2}}}{|NI|-1}\cdot(ni-1) \qquad \forall(m\in M,(t,kp)\in TKP,ni\in NI\wedge ni\neq 1) \tag{4.49}$$

$$q^{m,\mathrm{T,L3}}_{n,kp,t,ni} = q^{m,\mathrm{T,L3}}_{n,kp,t,ni=1} + \frac{q^{m,\mathrm{T,UP}}_{t} - q^{m,\mathrm{T,L3}}_{n,kp,t,ni=1}}{|NI|-1} \cdot (ni-1) \qquad \forall (n \in N, (t,kp) \in TKP, ni \in NI \wedge ni \neq 1) \tag{4.50}$$

Capital cost for technology *t* at L2 $(I^{\mathrm{T,L2}}_{m,kp,t,ni})$ and L3 $(I^{\mathrm{T,L3}}_{n,kp,t,ni})$ for each interval $ni \in NI$ is expressed using Equations (4.51) and (4.52):

$$I^{\mathrm{T,L2}}_{m,kp,t,ni} = I^{\mathrm{T,0}}_{t} \cdot \left(\frac{q^{m,\mathrm{T,L2}}_{m,kp,t,ni}}{q^{m,\mathrm{T,0}}_{t}}\right)^{sf} \qquad \forall (m \in M, (t,kp) \in TKP, ni \in NI) \tag{4.51}$$

$$I^{\mathrm{T,L3}}_{n,kp,t,ni} = I^{\mathrm{T,0}}_{t} \cdot \left(\frac{q^{m,\mathrm{T,L3}}_{n,kp,t,ni}}{q^{m,\mathrm{T,0}}_{t}}\right)^{sf} \qquad \forall (n \in N, (t,kp) \in TKP, ni \in NI) \tag{4.52}$$

where $I^{\mathrm{T,0}}_{t}$ is capital cost for the reference technology *t*, and sf is the scale factor, which is usually around 0.6 (the six-tenth rule) (You and Wang, 2011).

The slope of the line within each interval $ni \in NI$ is defined using Equation (4.53) for L2 $(m^{\mathrm{T,L2}}_{m,kp,t,ni})$ and Equation (4.54) for L3 $(m^{\mathrm{T,L3}}_{m,kp,t,ni})$:

$$m^{\mathrm{T,L2}}_{m,kp,t,ni} = \frac{I^{\mathrm{T,L2}}_{m,kp,t,ni+1} - I^{\mathrm{T,L2}}_{m,kp,t,ni}}{q^{m,\mathrm{T,L2}}_{m,kp,t,ni+1} - q^{m,\mathrm{T,L2}}_{m,kp,t,ni}} \qquad \forall (m \in M, kp \in KP, t \in T, ni \in NI \wedge ni \neq |NI|) \tag{4.53}$$

$$m^{\mathrm{T,L3}}_{m,kp,t,ni} = \frac{I^{\mathrm{T,L3}}_{n,kp,t,ni+1} - I^{\mathrm{T,L3}}_{n,kp,t,ni}}{q^{m,\mathrm{T,L3}}_{n,kp,t,ni+1} - q^{m,\mathrm{T,L3}}_{n,kp,t,ni}} \qquad \forall (n \in M, kp \in KP, t \in T, ni \in NI \wedge ni \neq |NI|) \tag{4.54}$$

The difference in capacity (the distance along the x-axis) is defined using Equation (4.55) for technology *t* at L2 and Equation (4.56) for technology *t* at L3 for this interval where binary variable ($y^{\mathrm{T,L2}}_{m,t,ni}$ and $y^{\mathrm{T,L3}}_{n,t,ni}$) is equal to 1.

$$\Delta q^{m,\mathrm{T,L2}}_{m,kp,t,ni} \leq (q^{m,\mathrm{T,L2}}_{m,kp,t,ni+1} - q^{m,\mathrm{T,L2}}_{m,kp,t,ni}) \cdot y^{\mathrm{T,L2}}_{m,t,ni} \qquad \forall (m \in M, (t,kp) \in TKP \wedge t \in T_2, ni \in NI \wedge ni < |NI|) \tag{4.55}$$

$$\Delta q^{m,\mathrm{T,L3}}_{n,kp,t,ni} \leq (q^{m,\mathrm{T,L3}}_{n,kp,t,ni+1} - q^{m,\mathrm{T,L3}}_{n,kp,t,ni}) \cdot y^{\mathrm{T,L3}}_{n,t,ni} \qquad \forall (n \in N, (t,kp) \in TKP \wedge t \in T_3, ni \in NI \wedge ni < |NI|) \tag{4.56}$$

Binary variable should be equal to 1 in at most one interval $ni \in NI \wedge ni < |NI|$:

$$\sum_{ni \in NI \wedge ni < |NI|} y^{\mathrm{T,L2}}_{m,t,ni} \leq 1 \qquad \forall (m \in M, t \in T_2) \tag{4.57}$$

$$\sum_{ni \in NI \wedge ni < |NI|} y^{\mathrm{T,L3}}_{n,t,ni} \le 1 \qquad \forall (n \in N, t \in T_3) \tag{4.58}$$

Maximal capacity for technology t at L2 ($q^{m,\mathrm{T,L2,UP}}_{m,pi,pm,t}$) and L3 ($q^{m,\mathrm{T,L3,UP}}_{n,pm,pp,t}$) is defined:

$$\sum_{(pi,t)\in PIT} \sum_{(pi,pm)\in PIPM} q^{m,\mathrm{T,L2,UP}}_{m,pi,pm,t} = \sum_{ni\in NI \wedge ni<|NI|} (q^{m,\mathrm{T,L2}}_{m,kp,t,ni} \cdot y^{\mathrm{T,L2}}_{m,t,ni} + \Delta q^{m,\mathrm{T,L2}}_{m,kp,t,ni}) \\ \forall (m \in M, (t,kp) \in TKP \wedge t \in T_2) \tag{4.59}$$

$$\sum_{(pm,t)\in PMT} \sum_{(pm,pp)\in PMPP} q^{m,\mathrm{T,L2,L3,UP}}_{n,pm,pp,t} = \sum_{ni\in NI \wedge ni<|NI|} (q^{m,\mathrm{T,L3}}_{n,kp,t,ni} \cdot y^{\mathrm{T,L3}}_{n,t,ni} + \Delta q^{m,\mathrm{T,L3}}_{n,kp,t,ni}) \\ \forall (n \in N, (t,kp) \in TKP \wedge t \in T_3) \tag{4.60}$$

Finally, the capital cost for each technology t at pre-processing and storage facilities m and process plants n is defined using Equations (4.61) and (4.62):

$$I^{\mathrm{T,L2}}_{m,t} = \sum_{(t,kp)\in TKP} \sum_{ni\in NI \wedge ni<|NI|} I^{\mathrm{T,L2}}_{m,kp,t,ni} \cdot y^{\mathrm{T,L2}}_{m,t,ni} + m^{\mathrm{T,L2}}_{m,kp,t,ni} \cdot \Delta q^{m,\mathrm{T,L2}}_{m,kp,t,ni}) \qquad \forall (m \in M, t \in T_2) \tag{4.61}$$

$$I^{\mathrm{T,L3}}_{n,t} = \sum_{(t,kp)\in TKP} \sum_{ni\in NI \wedge ni<|NI|} I^{\mathrm{T,L3}}_{n,kp,t,ni} \cdot y^{\mathrm{T,L3}}_{n,t,ni} + m^{\mathrm{T,L3}}_{n,kp,t,ni} \cdot \Delta q^{m,\mathrm{T,L3}}_{n,kp,t,ni}) \qquad \forall (n \in N, t \in T_3) \tag{4.62}$$

The sum of the storage, pre-treatment and operating cost and annual depreciation expense (c^{spod}) is given by the following Equation:

$$c^{\mathrm{spod}} = c^{\mathrm{stor}} + \sum_{pm\in PM} \sum_{t\in T} c^{\mathrm{pretreat,T}}_{pm,t} + \sum_{t\in T} c^{\mathrm{op,T}}_{t} + \sum_{m\in M} \sum_{t\in T} \frac{I^{\mathrm{T,L2}}_{m,t}}{ny} + \sum_{n\in N} \sum_{t\in T} \frac{I^{\mathrm{T,L3}}_{n,t}}{ny} \tag{4.63}$$

where ny is the number of project lifetime years.

4.2.1.4 Objective Function

The objective function maximises the annual profit before tax (P):

$$P = \sum_{n\in N} \sum_{(pp,t)\in PPT} \sum_{j\in J} \sum_{tp\in TP} q^{m,\mathrm{net,T,L3,L4}}_{n,t,j,pp,tp} \cdot c^{\mathrm{price}}_{pp,tp} + \sum_{m\in M} \sum_{j\in J} \sum_{pd\in PD} \sum_{tp\in TP} q^{m,\mathrm{L2,L4}}_{m,j,pd,tp} \cdot c^{\mathrm{price}}_{pd,tp} - \\ \sum_{i\in I} \sum_{pi\in PI} \sum_{tp\in TP} q^{m,\mathrm{L1}}_{i,pi,tp} \cdot c^{\mathrm{cost}}_{pi} - \sum_{m\in M} \sum_{t\in T} \sum_{pbuy\in PBUY} \sum_{tp\in TP} q^{m,\mathrm{buy,L2}}_{m,t,pbuy,tp} \cdot c^{\mathrm{cost}}_{pbuy} - \\ \sum_{n\in N} \sum_{t\in T} \sum_{pbuy\in PBUY} \sum_{tp\in TP} q^{m,\mathrm{buy,L3}}_{n,t,pbuy,tp} \cdot c^{\mathrm{cost}}_{pbuy} - c^{\mathrm{tr}} - c^{\mathrm{spod}} \tag{4.64}$$

The income in Equation (4.64) represents the revenues from selling produced (first term) and direct products (second term). The outcome – Equation (4.64) – represents the raw material cost (third term), cost for purchased raw materials at L2 (fourth term), and at L3 (fifth term), transportation cost (sixth term), and storage, pre-treatment and operating cost, and annual depreciation expense (seventh term).

4.2.2 Illustrative Example

The four layer (L1-L4) supply chain network superstructure (see Figure 4-3) and the presented model are applied, in order to perform the synthesis of the optimally-integrated biorefinery.

A multi-period optimisation model of a heat-integrated biorefinery's supply network is applied within the illustrative example over a small region. The objective of the synthesis is to maximise the economic performance of the biofuels' supply network involving bioethanol, biodiesel, FT-diesel, hydrogen, and green gasoline. A set of biomass feedstocks is defined that can be converted into biofuels. It includes food-based crops (corn grain, wheat), agricultural residues (corn stover, wheat straw), energy crop (switchgrass), and wood residues (forest thinning). Furthermore, the use of waste cooking oil and algae is considered for the production of biodiesel.

A number of transformation technologies for converting biomass and waste to biofuels (Martín and Grossmann, 2013) are considered, such as i) the dry-grind process (corn grain, wheat), ii) gasification and catalytic synthesis and iii) gasification and syngas fermentation (corn stover, wheat straw, switchgrass, forest thinning), iv) biochemical conversion of lignocellulosic biomass (switchgrass), v) FT-diesel and green gasoline production (corn stover, wheat straw, switchgrass, forest thinning), vi) hydrogen production (corn stover, wheat straw, switchgrass, forest thinning), and vii) biodiesel production (algae, waste cooking oil).

Figure 4-4 presents the general superstructure of the analysed supply chain.

Food-based products can be either directly used at demand locations, without transforming them to biofuels, or transformed within biorefineries into biofuels and other bioproducts.

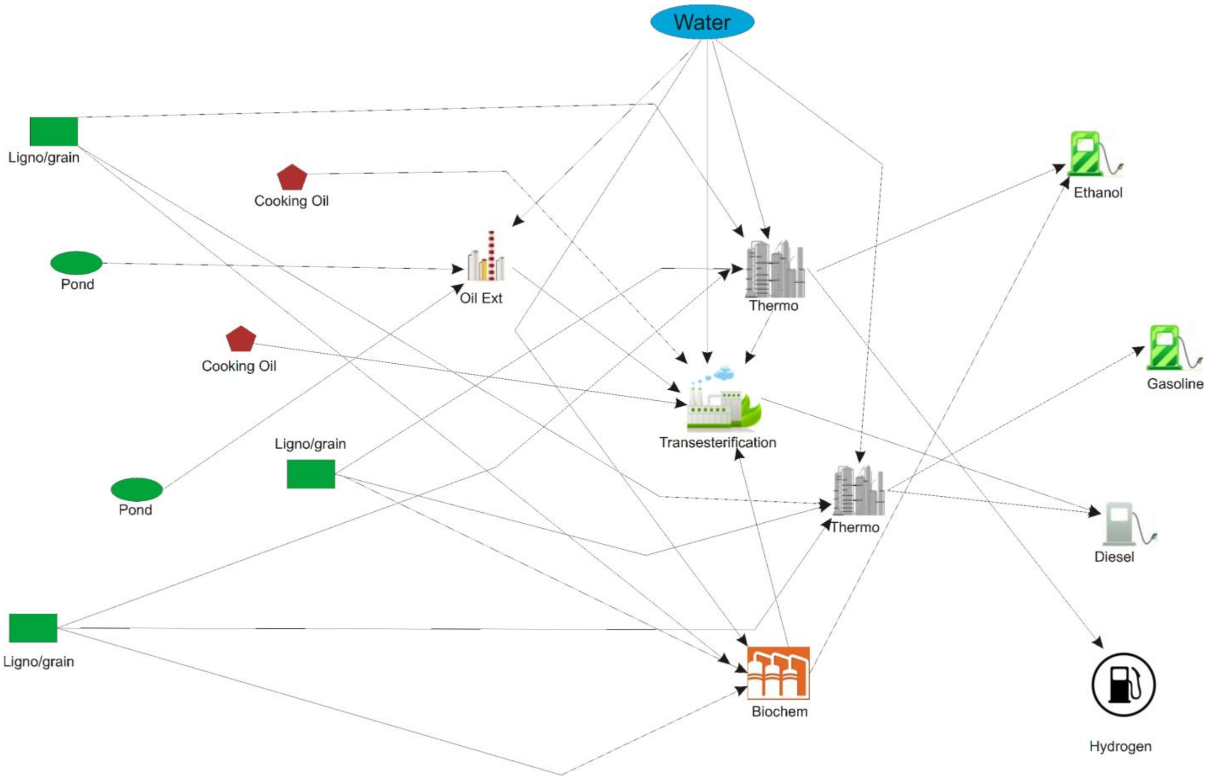


Figure 4-4. General superstructure of the supply network (Čuček et al., 2013c)

The structure of the demonstration supply chain network is illustrated in Figure 4-5. The region is divided into 16 zones, each zone with an area of 2,000 km^2 (40 km × 50 km). The total area of the region is 32,000 km^2. The locations of the zones are shown using black circles, with the red rectangles the possible locations of collection centres and biorefineries, and with the blue stars indicating the locations of regional demand. Population density within the region is assumed to be 100 inhabitants per km^2 (population of 3,200,000).

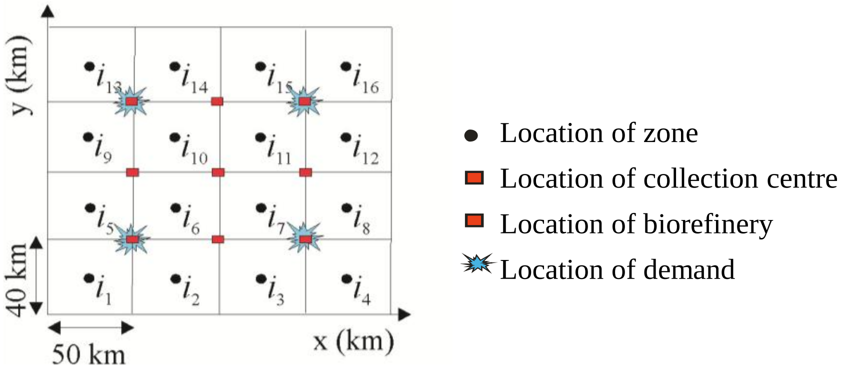


Figure 4-5. Regional plan covering 16 zones (Čuček et al., 2013b)

It is assumed that up to 20 % of the total area of each zone could be dedicated to biofuels, either by deforestation or by intensification, in order to be on the safe side regarding food production and to avoid biodiversity loss. For simplification it is assumed, that in each zone the same amount of each biomass can be grown, however altogether the cultivation area for biomass devoted for biofuels cannot exceed a specific percentage (from 2 % up to 20 %) of the land area in each zone. The only restrictions for the model are the availability of a cultivation area for biofuels and food, and maximum and minimum capacities for the technologies.

4.2.2.1 Harvesting and Supply

A set of biomass feedstocks and wastes that can be grown or collected in each zone is defined. It includes corn grain, corn stover, wheat, wheat straw, switchgrass, forest thinning, waste cooking oil and algae. Corn grain, corn stover, wheat, wheat straw, switchgrass and forest thinning are seasonal raw materials, and their harvesting period can be seen in Table 4-1. Waste cooking oil and algae are year-round raw materials, and are available during the whole year.

Again it is assumed that from the entire corn plant, around 50 % is grain and 50 % stover, and it is possible to remove around 60 % of stover from the fields. From the wheat fields it is assumed that the residue/crop (wheat straw/wheat grain) ratio is 1.7 for winter wheat (Nelson, 2002), and 60 % of the straw is possible to remove to maintain long-term soil fertility and minimise erosion. Crop residues and switchgrass are dried on the fields, and once dried, they are collected in round or square bales.

Forest residues consist of small trees, branches and tops left within the harvest areas, after the thinning, cleaning or final felling of forest stands, and are residues from softwood, hardwood and decay-damaged wood (Gunnarsson et al., 2004). Harvesting is done in autumn and winter months (Vonk and Theunissen, 2007), and the residues are dried during the summer. Once the residues are dried, they are forwarded and collected into piles within the storage sites.

The quantity of waste cooking oil generated per year is in the order of several kg per person in industrialised countries. An estimate of the potential amount of waste cooking oil collected in the EU is from 700 kt to 1 Mt/y (Kulkarni and Dalai, 2006). Estimates of collectable waste cooking oil vary from 5 to 13 kg per capita per year (Rice et al., 1997). 10 kg of waste cooking oil per capita per year is assumed in this study.

It is assumed that algae are grown, harvested, and dried near the collection and pre-processing facilities. Algae oil extraction is also accomplished at the pre-processing locations also. The monthly algal productivity trend is taken from (Jiménez et al., 2003), where the algal yield is the highest in summer (2,589 t/km^2 in July), and the lowest in winter months (371.3 t/km^2 in January). Algal yield increases with increasing the temperatures, thus higher productivity is obtained at higher temperatures (Jiménez et al., 2003).

Characteristics of biomass and waste resources are specified in Table 4-1.

Table 4-1. Characteristics of the raw materials

	Yield	Moisture (%)		Bulk density	Price ($/t)		Harvesting period
	(t/(km^2·y))	wet	dry	(kg/m^3)	wet	dry	
Corn grain	730	15-30	15	720	250	300	September – November
Wheat	350	-	13.5	800	-	330	May – July
Corn stover	440	20-64	15	145	-	60	September – November
Wheat straw	350	9-25	15	140	-	60	May – July
Switchgrass	1,000	12-70	15	160	-	30	August – October
Forest residues	350	45	20	300	25	40	July – March
Algae	18,250	-	5	918*	-	61	Whole year
Waste cooking oil	1	-	0.25	924	-	200	Whole year

*density of algal oil

Some of the raw materials should be purchased from the market, such as hydrogen and ethanol, if they are not produced and recycled within the region. Hydrogen is used for FT-diesel and green gasoline production. Methanol and/or ethanol are used as raw materials for biodiesel production. The quantities of the sum of purchased and recycled raw materials (additional raw material) in regard to produced key products ($kg_{\text{additional raw material}}/kg_{\text{key product}}$) required for specific process technology, are presented in Table 4-2.

4.2.2.1 Collection, Pre-Processing, and Storage

It is assumed that all biomass feedstocks are collected and stored in centralised covered collection and pre-processing centres. Collection centres and terminals are used to balance the seasonal fluctuation in production and supply of biomass feedstocks, and the demand. Once they are demanded for energy production, they are transported to the biorefinery. Corn grain usually has high moisture content, and therefore it should be dried, which is required for safe storage. Forest residues can be densified by chipping, grinding, or bundling to reduce the transportation and subsequent operating cost. Chipping is the most efficient and least expensive method (Schnepf, 2010). It is assumed that forest residues are chipped at terminals, before being transported to biorefineries (Gunnarsson et al., 2004).

Table 4-2. Characteristics of additional raw materials

	Price ($/t)	Quantity (t/t)	Key product	Technology
Ethanol	1,745*	0.1156	Biodiesel	Transesterification of oil with ethanol
Methanol	280	0.1156	Biodiesel	Transesterification of oil with methanol
Hydrogen	1,580	0.0116	FT-diesel	Gasification, FT synthesis and hydrocracking

*assumed that ethanol price is same with gasoline price in regards to calorific value. Gasoline price is taken from Wikipedia (Wikipedia, 2012a), and gasoline higher calorific value (HCV) (47.3 MJ/kg) from The Engineering ToolBox (The Engineering Toolbox, 2013)

Waste cooking oil should be treated to remove impurities, such as dirt, food remains, water, free fatty acids, odor, etc. The growth of microalgae can be carried out in open ponds (extensive ponds and artificial raceway ponds) or in photobioreactors (closed systems). For this study, the raceway ponds are selected to grow algae, because they are widely used systems for large-scale outdoor microalgae cultivation, and because they are cheaper, easier to build and to operate, and have low energy inputs (Brennan and Owende, 2010). Next, the algae are harvested to eliminate the water that accompanies them, which can be recycled, using screening, thickening, dewatering, and drying (Martín and Grossmann, 2012b). It is assumed that once the algae are dried they are shipped to pre-processing facilities for oil extraction. Algal oil is usually obtained using mechanical cell disruption, followed by solvent extraction (Martín and Grossmann, 2012b). In this work the hexane solvent extraction is considered along with the oil press/expeller method. After the oil has been extracted using an expeller, the pulp is mixed with cyclohexane to extract the remaining oil content (Martín and Grossmann, 2012b). The oil dissolves in cyclohexane, and the pulp is filtered from the solution. The oil and cyclohexane are separated by means of distillation. 50 % lipid content of dry cell weight is assumed (Weyer et al., 2010).

Furthermore, the harvesting losses and deterioration of biomass feedstock over time because of storage is assumed in this study, and is presented in Table 4-3. Costs of pre-processing and storage are also shown in Table 4-3.

Table 4-3. Cost of the pre-processing and storage, and the biomass deterioration percentage

	Corn grain	Wheat	Corn stover	Wheat straw	Switch-grass	Forest residues	Algal oil	Waste cooking oil
Storage ($/t) – dry	17	17	11	11	11	10	10	10
Drying ($/t)	16	0	0	0	0	0	0	0
Chipping ($/t)	0	0	0	0	0	15	0	0
Mechanical cleaning ($/t)	0	0	0	0	0	0	0	30
Additional treatment ($/t)	0	0	0	0	0	0	0	60
Oil extraction ($/t)	0	0	0	0	0	0	131*	0
Harvesting loss (%)	3	3	5	5	5	5	0	0
Deterioration (%/month)	0.5	0.5	0.5	0.5	0.5	0.5	0	0

*cost for algal oil production, including algae growing, harvesting and oil extraction

4.2.2.1 Main Processing

Several process technologies are considered, such as the dry-grind process, gasification and catalytic synthesis, gasification and syngas fermentation, biochemical conversion of lignocellulosic biomass, FT-diesel and green gasoline production, hydrogen production and biodiesel production.

The dry-grind process

The dry-grind process is briefly described in Section 3.1 (see Figure 3-2). It should be noted, that the dry-grind process can be applied for different cereals, corn, wheat, barley, rye, and others (Singh, 2008).

Gasification and further catalytic synthesis or syngas fermentation

The gasification and further catalytic synthesis and gasification and further syngas fermentation are also briefly described in Section 3.1 (see Figure 3-3). Different lignocellulosic raw materials can be used, such as crop residues (corn stover, wheat straw), switchgrass, wood chips, hybrid poplar, etc. (Phillips et al., 2007).

Biochemical conversion of lignocellulosic biomass

An optimal conceptual design for ethanol production via the hydrolysis of switchgrass by postulating a superstructure that embeds two pre-treatment alternatives, ammonia fibre explosion (AFEX) and dilute acid pre-treatment, was proposed by (Martín and Grossmann, 2012a). Before hydrolysis, the structure of the switchgrass should be broken to allow contact between the polymers and the enzymes. Pre-treatment is followed by hydrolysis of the biomass, fermentation of the sugars, mainly glucose and xylose, using *Zymomonas mobilis* bacteria into ethanol, different acids and other by-products, and finally dehydration of ethanol by means of a beer column followed by molecular sieves to fuel grade quality. The lignin is used to obtain energy for the process. HI is also performed.

The optimal flowsheet uses dilute acid pre-treatment, which is cheaper and more environmentally-friendly since it consumes less energy and requires less cooling water. Figure 4-6 shows the flowsheet based on the optimal hydrolysis process. It should be noted, that only switchgrass is used as a raw material, since the hydrolytic path is sensitive to the composition of lignocellulosic biomass and it is difficult to mix different biomass feedstocks together (Martín and Grossmann, 2013).

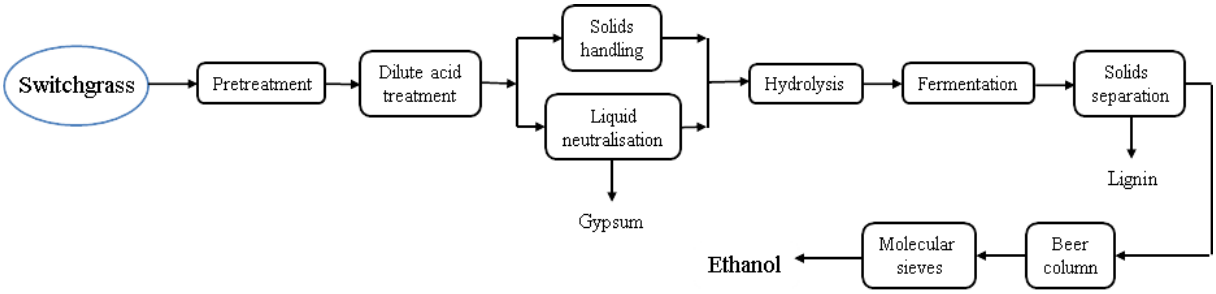


Figure 4-6. Hydrolysis-based production process of ethanol from switchgrass (modified from (Martín and Grossmann, 2013))

FT-diesel and green gasoline production

A superstructure embedding alternative technology for the optimisation of FT-diesel and green gasoline production process from switchgrass has been proposed by (Martín and Grossmann, 2011c). The optimal process starts with the indirect gasification of the biomass. The gas obtained is reformed, cleaned-up, and its composition may be adjusted in terms of the ratio CO/H_2 for the optimal production of the diesel fraction. Next, the removals of CO_2 and H_2S are performed by means of two clean-up processes such as absorption in MEA and PSA. Then the FT-reaction is conducted and the products are separated. Hydrocracking of the heavy products is also considered to increase the yield towards diesel. Also energy integration is performed. Figure 4-7 illustrates the optimal flowsheet for the production of FT-diesel. It should be noted, that besides switchgrass, other lignocellulosic raw materials can be used for FT-diesel production using this technology.

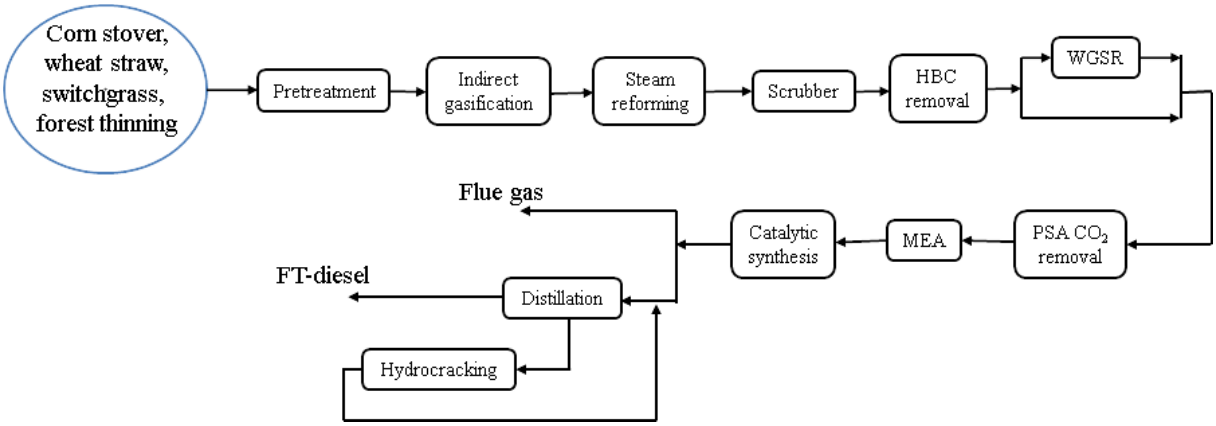


Figure 4-7. Optimal flowsheet for the production of FT-diesel (modified from (Martín and Grossmann, 2013))

Hydrogen production

The conceptual design for hydrogen production from switchgrass has been addressed by (Martín and Grossmann, 2011b). The optimal process embeds indirect gasification technology, steam reforming, gas cleaning and a water gas shift reactor (WGSR) with membrane separation. Pure hydrogen is obtained. Further energy is then integrated. Figure 4-8 presents the block flowsheet diagram for the process. The disadvantage of using biomass to obtain hydrogen is that the biomass fixes carbon from the atmosphere, and thus it should be considered as a source of carbon too, not only a source of hydrogen. This fact can be alleviated if the CO_2 generated is injected into the ponds or photoreactors for the production of microalgae (Martín and Grossmann, 2013). Different lignocellulosic raw materials can be used, such as crop residues, switchgrass, wood chips, etc.

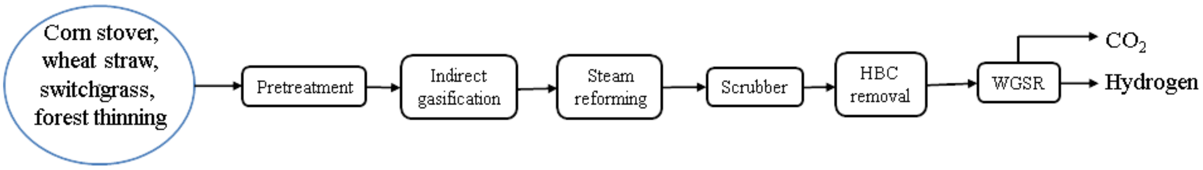


Figure 4-8. Optimal flowsheet for the production of hydrogen (modified from (Martín and Grossmann, 2013))

Biodiesel production

The conceptual design for the production of biodiesel from cooking oil and algae oil was proposed by (Martín and Grossmann, 2012b), and later extended to the use of bioethanol as transesterifying agent in (Severson et al., 2013). In terms of the optimal process, the best technology for transferring algal oil to biodiesel is homogeneous alkali-catalysed transesterification, whilst for waste cooking oil the best is heterogeneous-catalysed transesterification. The stream coming out of the reactors is treated to recover the methanol by means of a distillation column. The bottoms are sent to purification including neutralisation, phase separation, and biodiesel and glycerol purification. HI of the process is also performed (Duran and Grossmann, 1986). Figure 4-9 presents the block diagram for biodiesel production.

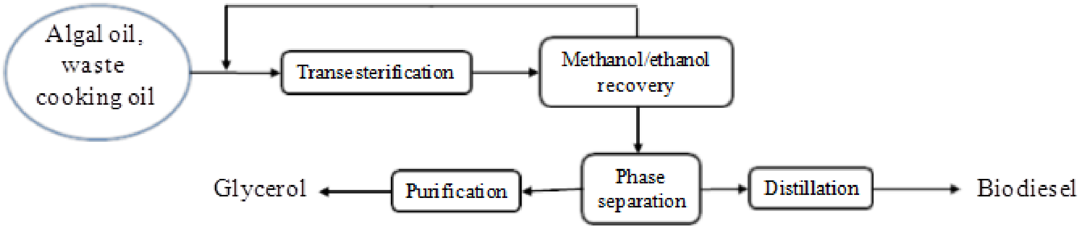


Figure 4-9. Biodiesel production scheme (modified from (Martín and Grossmann, 2013))

Summary of data related to main processing

Table 4-4 and Table 4-5 present the summary of the main features for the optimised processes at their reference capacities, obtained from the detailed models (Martín and Grossmann, 2013) Table 4-4 shows the data for the optimised reference processes relating to converting cereals and lignocellulosic raw materials into biofuels, and Table 4-5 the data relating to biodiesel production.

Table 4-4. Main features relating to ethanol, FT-diesel and hydrogen production

	Main product	Ethanol	Ethanol	Ethanol	Ethanol	FT-Diesel	H_2
	Production technology*	BPLB	DGP	GCS	GSF	FTDP	H2P
Investment (M$)		169	86	335	260	216	148
Capacity (kt/y)		183.97	183.97	183.97	183.97	193.055	60
Biofuel yield (kg/kg$_{wet}$)		0.28	0.32	0.20	0.33	0.19	0.11
Production cost ($/kg)**		0.26	0.40	0.13	0.26	0.22	0.68
Water consumption (L/L)		1.66	1.5	0.36	1.59	0.15	-
Energy consumption (MJ/kg)		-3.32	7.60	-3.10	8.87	-18.61	-3.84
By-product (kg/kg$_{biomass}$)	H_2	0	0	0.029	0.035	-0.0022	0
	Gasoline	0	0	0	0	0.0504	0
	Flue gas	0	0	0	0	0.086	0
	Mix alcohol	0	0	0.031	0	0	0
	DDGS	0	0.23	0	0	0	0
	Lignin	0.181	0	0	0	0	0

*BPLB – Biochemical conversion of lignocellulosic biomass, DGP – the dry-grind process, GCS – gasification and further catalytic synthesis, GSF – gasification and further syngas fermentation, FTDP – FT-diesel and green gasoline production, H2P – hydrogen production

**production costs include cost for raw materials, utilities, equipment, chemicals and other costs

Table 4-5. Main features relating to reference biodiesel production

Main product	Algal oil	Biodiesel	Biodiesel	Biodiesel	Biodiesel
Main raw materials	Algae	Cooking oil, methanol	Cooking oil, ethanol	Algal oil, methanol	Algal oil, ethanol
Total investment (M$)	93	17	19	17	19
Capacity (kt/y)	243.25	239.84	239.84	229.85	229.85
Biofuel yield (kg/kg$_{oil}$)	0.5	0.96	0.96	0.96	0.96
Production cost ($/kg)*	0.07	0.20	0.20	0.13	0.13
Water consumption (L/L)	0	0.33	0.33	0.60	0.60
Energy consumption (MJ/kg)	0.35	0.58	0.58	0.58	0.58
By-product glycerol (kg/kg$_{oil}$)	0.108	0.108	0.102	0.108	0.102

*production costs include cost for raw materials, utilities, equipment, chemicals and other costs

In order to calculate capital costs of the processing technologies at different capacities, a capacity exponent (*sf*) of 0.6 is considered (You and Wang, 2011). The scaling equation is:

$$I_t^{\mathrm{T}} = I_t^{\mathrm{T},0} \cdot \left(\frac{q_t^{m,\mathrm{T}}}{q_t^{m,\mathrm{T},0}} \right)^{0.6} \tag{4.65}$$

where I_t^{T} stands for the capital cost of technology *t* at layer L*b*, and $q_t^{m,\mathrm{T}}$ for the capacity of technology *t* at L2 and L3. The reference capital cost and capacities ($I_t^{\mathrm{T},0}$ and $q_t^{m,\mathrm{T},0}$) are shown in Table 4-4 and Table 4-5. The capacities of the plants ($q_t^{m,\mathrm{T}}$ – $q_{m,pi,pm,t}^{m,\mathrm{T,L2,UP}}$ and $q_{n,pm,pp,t}^{m,\mathrm{T,L3,UP}}$) can be within the range of $0.5 \cdot q_t^{m,\mathrm{T},0} \le q_t^{m,\mathrm{T},0} \le 3 \cdot q_t^{m,\mathrm{T},0}$.

Table 4-6 presents the operating cost ($c_{p,t}^{\text{op,T}}$) of different processing technologies. It should be noted that within the model only first part of the cost presented in Table 4-6 is included, since the cost of biomass resources, additional raw materials for conversion (such as methanol, ethanol and hydrogen), utilities and byproducts prices are separately included.

Table 4-6: Operating costs of the processing technology

Technology	Operating cost ($/gal*)
Biochemical conversion of lignocellulosic biomass	$0.4911-0.013\cdot\frac{c_{\text{Steam}}^{\text{cost}}}{c_{\text{Steam}}^{\text{cost,0}}}+0.3166\frac{c_{\text{Switchgrass}}^{\text{cost}}}{c_{\text{Switchgrass}}^{\text{cost,0}}}$
Dry-grind process	$0.3582+0.0908\cdot\frac{c_{\text{Steam}}^{\text{cost}}}{c_{\text{Steam}}^{\text{cost,0}}}+0.791\frac{c_{\text{Cereal}}^{\text{cost}}}{c_{\text{Cereal}}^{\text{cost,0}}}-0.178\frac{c_{\text{DDGS}}^{\text{cost}}}{c_{\text{DDGS}}^{\text{cost,0}}}$
Gasification and syngas fermentation	$0.4578+0.2744\cdot\frac{c_{\text{Steam}}^{\text{cost}}}{c_{\text{Steam}}^{\text{cost,0}}}+0.3425\frac{c_{\text{Lignocellulosic}}^{\text{cost}}}{c_{\text{Lignocellulosic}}^{\text{cost,0}}}-0.4514\frac{c_{\text{H}_2}^{\text{cost}}}{c_{\text{H}_2}^{\text{cost,0}}}$
Gasification and catalytic synthesis	$0.6249-0.0248\cdot\frac{c_{\text{Steam}}^{\text{cost}}}{c_{\text{Steam}}^{\text{cost,0}}}+0.4436\frac{c_{\text{Lignocellulosic}}^{\text{cost}}}{c_{\text{Lignocellulosic}}^{\text{cost,0}}}-0.636\frac{c_{\text{H}_2}^{\text{cost}}}{c_{\text{H}_2}^{\text{cost,0}}}$
Gasification, FT synthesis and hydrocracking	$0.608+0.411\frac{c_{\text{Lignocellulosic}}^{\text{cost}}}{c_{\text{Lignocellulosic}}^{\text{cost,0}}}+0.0298\frac{c_{\text{H}_2}^{\text{cost}}}{c_{\text{H}_2}^{\text{cost,0}}}-0.323\cdot\frac{c_{\text{Steam}}^{\text{cost}}}{c_{\text{Steam}}^{\text{cost,0}}}$
Gasification and hydrogen production	$0.4336-0.0215\cdot\frac{c_{\text{Steam}}^{\text{cost}}}{c_{\text{Steam}}^{\text{cost,0}}}+0.3166\frac{c_{\text{Lignocellulosic}}^{\text{cost}}}{c_{\text{Lignocellulosic}}^{\text{cost,0}}}$
Transesterification of cooking oil with methanol	$0.1288+0.629\frac{c_{\text{Oil}}^{\text{cost}}}{c_{\text{Oil}}^{\text{cost,0}}}-0.201\frac{c_{\text{Glycerol}}^{\text{cost}}}{c_{\text{Glycerol}}^{\text{cost,0}}}+0.098\frac{c_{\text{Methanol}}^{\text{cost}}}{c_{\text{Methanol}}^{\text{cost,0}}}+0.0096\cdot\frac{c_{\text{Natural gas}}^{\text{cost}}}{c_{\text{Natural gas}}^{\text{cost,0}}}$
Transesterification of algal oil with methanol	$0.108+0.418\frac{c_{\text{Oil}}^{\text{cost}}}{c_{\text{Oil}}^{\text{cost,0}}}-0.218\frac{c_{\text{Glycerol}}^{\text{cost}}}{c_{\text{Glycerol}}^{\text{cost,0}}}+0.110\frac{c_{\text{Methanol}}^{\text{cost}}}{c_{\text{Methanol}}^{\text{cost,0}}}+0.0095\cdot\frac{c_{\text{Natural gas}}^{\text{cost}}}{c_{\text{Natural gas}}^{\text{cost,0}}}$
Transesterification of cooking oil with ethanol	$0.1435+0.426\frac{c_{\text{Oil}}^{\text{cost}}}{c_{\text{Oil}}^{\text{cost,0}}}-0.201\frac{c_{\text{Glycerol}}^{\text{cost}}}{c_{\text{Glycerol}}^{\text{cost,0}}}+0.162\frac{c_{\text{Ethanol}}^{\text{cost}}}{c_{\text{Ethanol}}^{\text{cost,0}}}+0.0096\cdot\frac{c_{\text{Natural gas}}^{\text{cost}}}{c_{\text{Natural gas}}^{\text{cost,0}}}$
Transesterification of algal oil with ethanol	$0.1435+0.426\frac{c_{\text{Oil}}^{\text{cost}}}{c_{\text{Oil}}^{\text{cost,0}}}-0.201\frac{c_{\text{Glycerol}}^{\text{cost}}}{c_{\text{Glycerol}}^{\text{cost,0}}}+0.162\frac{c_{\text{Ethanol}}^{\text{cost}}}{c_{\text{Ethanol}}^{\text{cost,0}}}+0.0096\cdot\frac{c_{\text{Natural gas}}^{\text{cost}}}{c_{\text{Natural gas}}^{\text{cost,0}}}$
Oil extraction	$0.122+0.005\cdot\frac{c_{\text{Steam}}^{\text{cost}}}{c_{\text{Steam}}^{\text{cost,0}}}$

*for gasification and hydrogen production instead of gal, kg is used

Integration possibilities

In Figure 4-10 the integration possibilities between the different processes presented before can be seen in terms of energy, intermediates and final products.

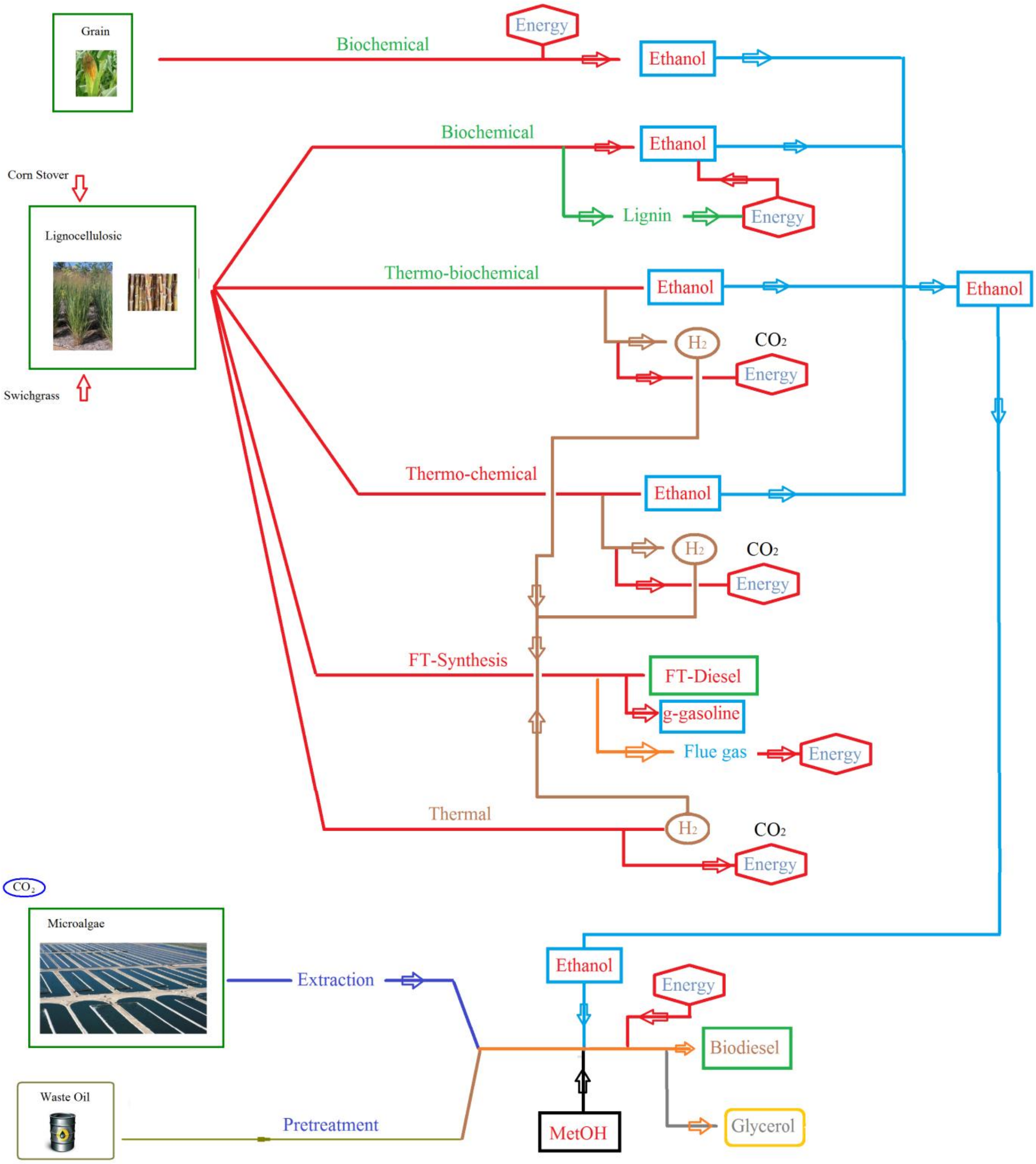


Figure 4-10. Integration possibilities (Čuček et al., 2013c)

The hydrogen and ethanol are needed within processes such as the FT-diesel and green gasoline production or the biodiesel production, whilst some processes generate energy that can be used within other processes. The supply chain model evaluates these possibilities in a systematic way.

4.2.2.1 Consumption

Except within the last scenario (see Section 4.2.3.5), it is assumed that the demand for biofuels exceeds production, and therefore all the produced biofuels, by-products, and food are consumed within the region. It is assumed that produced products can be stored on site, if it is more profitable to sell them in other time period as produced, and there is enough production in this time period to satisfy the demand. The prices, bulk densities and HCVs for the products are presented in Table 4-7.

Table 4-7. Characteristics of products

	Ethanol	Biodiesel	FT-diesel	H_2	Green gasoline*	DDGS	Glycerol	Lignin
Price ($/ton)	1,745**	1,758**	2,000	1,580	2,778	170	600	0***
Bulk density (kg/m^3)	810	880	850	0.09	720	500	1261	550
HCV (MJ/kg)	29.7	40	45.5	141.8	47.3	6.3	19	26

*assumed that properties are the same as that of gasoline

**assumed that ethanol price is the same as gasoline price, and biodiesel price as this of petroleum diesel price in regards to HCV (calorific values are 47.3 MJ/kg for gasoline, and 44.8 MJ/kg for diesel (The Engineering Toolbox, 2013))

***assumed to be zero to be on the conservative side

4.2.2.1 Transportation

Road transport (by truck) is the major transportation mode for shipping biomass feedstocks (You et al., 2012). Trucks dominate bulk agricultural commodity deliveries if the distances are less than 500 km (Searcy et al., 2007). Since lignocellulosic biomass has relatively low transportation density, both volume and weight capacities should be considered during transportation (You et al., 2012), however mass is usually a primary factor when setting the shipment (Searcy et al., 2007). On average, 26 t is the capacity for such trucks that transport cereals (Meyer, 2004), around 20 t is the capacity of flatbed trucks that transport crop residues and switchgrass (Bransby et al., 2008), and around 40 t is the capacity of each chip van that transports chipped forest residue (Searcy et al., 2007). Liquids (waste cooking oil, algal oil, biodiesel, ethanol, FT-diesel, and green gasoline) are transported in cistern lorries with capacities of 7,500 to 32,000 L (Talens Peiró, 2006), or in tandem tankers with capacities of 40 t (Searcy et al., 2007). Hydrogen can be distributed to storage facilities or to refuelling stations using compressed gas trucks, liquid hydrogen tanker trucks, and metal hydride truck. The net delivered capacities of the compressed gas trucks are around 240 kg (Yang and Ogden, 2007) – 280 kg (Parker, 2007) of hydrogen per load, and capacities of liquid tanker trucks are around 4 t (Paster, 2006). Alternatively all products can be transported by rail and ship if the distances between locations of source and usage are far away. Liquid fuels and hydrogen can also be transported by pipelines.

Transportation costs consist of distance fixed cost (cost of loading and unloading) and distance variable cost (mostly fuel cost) (Searcy et al., 2007). Loading and unloading costs include the equipment and labour needed to load and unload biomass feedstocks and bioproducts (Thompson and Tyner, 2012). Additional costs are: the amortised capital cost of the truck, operating costs which include labour, maintenance, insurance, and repairs (Miranowski, 2010). Table 4-8 summarises the transportation cost.

Table 4-8. Transportation cost

Raw material	Distance fixed cost ($/t)	Distance variable cost ($/(t·km))	Product	Distance fixed cost ($/t)	Distance variable cost ($/(t·km))
Corn grain	6.3	0.07	Ethanol	3.86	0.05
Wheat	6.3	0.07	Biodiesel	3.86	0.05
Corn stover	8.5	0.255	FT-diesel	3.86	0.05
Wheat straw	8.5	0.255	Hydrogen	-	0.8
Switchgrass	8.5	0.255	Green gasoline	3.86	0.05
Forest residue	10	0.348	DDGS	6.3	0.07
Algal oil	3.86	0.05	Glycerol	6.3	0.07
Waste cooking oil	3.86	0.05	Lignin	6.3	0.07

Utilities are transported between technologies, and between technologies and demand locations via pipelines. The pipelines costs are capital costs for district heating network, including pipes and related equipment (Kapil et al., 2012). The pipelines costs are treated with binary variables whether pipeline link exist or not (Parker, 2007). It is assumed that district heating network costs 1,460 $/m, and also that 1 % of the heat is lost per km in transportation (Kapil et al., 2012). If the source and sink of the heat energy are at the same plant location, the distance between those locations of 1 km is assumed.

4.2.3 Results and Discussion

The mathematical model presented in Section 4.2.1 is applied on an illustrative example of a smaller region with 16 zones (area of 32,000 km^2) – see Figure 4-5. The model of this illustrative example consists of approximately 460,000 constraints, 1,000,000 single variables, and 2,400 binary variables. MILP is performed using GAMS (GAMS Development Corporation, 2010) and a GUROBI solver on a personal computer with an Intel® Core™ i7-2600 processor with 16 GB of RAM.

Several scenarios are considered, all with 12 time periods (12 months) and with intermediate storage at L2 and L3.

4.2.3.1 First Scenario

During the first scenario, the area available for all raw materials is constant throughout the year. Seasonal raw materials (corn and wheat, and forest residue) could be harvested over optimal time period(s). Perennial energy crop switchgrass is also considered as a seasonal raw material within the model, since it is harvested seasonally. Switchgrass can be harvested twice a year, however in this study only one cut per year is assumed with harvesting period from August to October (Kumar and Sokhansanj, 2007). The results from this scenario can be seen in Table 4-9. The discussion of the results comes together with those of the second scenario.

4.2.3.2 Second Scenario

During the second scenario, the selected area for year-round raw materials could be different for each month (algae and waste cooking oil). Seasonal raw materials (corn and wheat), and switchgrass and forest residue could be harvested over optimal time period(s).

The main results from the first two scenarios are presented in Table 4-9. In the first and second scenarios, it is assumed that up to 10 % of the total area of each zone could be dedicated to biofuels.

Table 4-9. Main results from optimisation

	First scenario	Second scenario
Profit	7,210 M$/y	10,244 M$/y
Raw materials	Algae: 7,713 kt/y Switchgrass: 2,777 kt/y	Algae: 12,709 kt/y Switchgrass: 929 kt/y
Technologies	- Gasification and syngas fermentation - Biodiesel production from algal oil with methanol	- Gasification and syngas fermentation - Biodiesel production from algal oil with methanol
Investment cost	4,000 M$	2,351 M$
Production cost	1,224 M$/y	1,459 M$/y
Transportation cost	112 M$/y	107 M$/y
Water consumption	4,212 kt/y	4,721 kt/y
Biofuels	Biodiesel: 3,702 kt/y Bioethanol: 857 kt/y Hydrogen: 91 kt/y	Biodiesel: 6,100 kt/y Bioethanol: 286 kt/y Hydrogen: 30 kt/y
Solution time	2,558 CPU-s	1,358 CPU-s
Optimality gap	1.9 %	1.1 %

It can be seen from the results that the profit is much higher for those cases when not all of the available year-round raw materials are used for bioenergy (10,244 M$/y vs. 7,210 M$/y). The most profitable operations involve the usages of algal biomass and switchgrass as raw materials due to the highest yield. The selected technologies are gasification and further syngas fermentation, and the transesterification of the algal oil with methanol. During the second scenario it could be seen that more algal biomass and less switchgrass is used, and the investment cost is significantly lower (2,351 M$ vs. 4,000 M$). The amount of biodiesel produced is much higher whilst the bioethanol and hydrogen, which are produced within the same process, are much lower when the selected area for year-round raw materials could be different during each month.

Additionally, the storage capacities can be seen on Figure 4-11a for the algal oil, and on Figure 4-11b for the switchgrass.

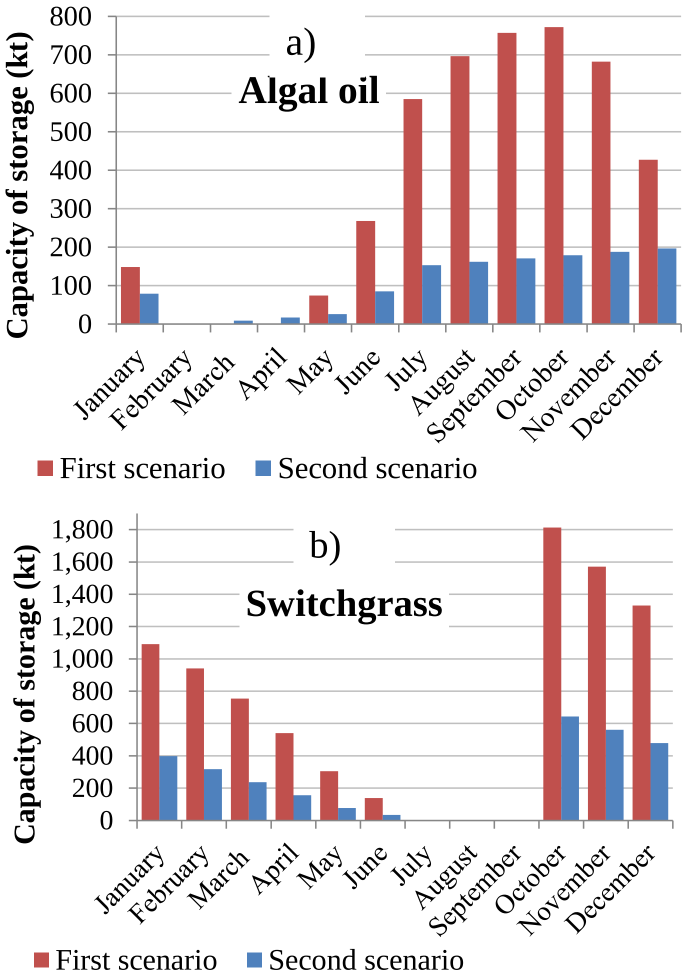


Figure 4-11. Storage capacities for a) algal oil, b) switchgrass (Čuček et al., 2013c)

The first scenario requires 2,777.3 km^2 of land devoted for switchgrass, and only 422.7 km^2 for algae, and the second scenario requires only 929.1 km^2 of land devoted for switchgrass, and 2,270.9 km^2 for algae. It can be seen that the scenario with constant area (first scenario) requires more than three times larger storage capacities for algal oil and switchgrass compared to the scenario with variable area (second scenario). It is assumed that switchgrass could be harvested only from August to October over optimal time periods, and therefore switchgrass is stored for several months in order to ensure continuous production to lower the capital cost. However, the storage capacities are limited due to biomass degradation during storage, and storage cost. Therefore, there is a trade-off between duration of storage and storage capacity, and the capital cost. Higher storage capacity for switchgrass is required during the first scenario since more switchgrass is grown and used as during the second scenario.

Also for algae there is a trade-off between storage costs and capital costs in order to ensure continuous production. The storage capacity for algae is the highest in summer and autumn, since in summer months the yield of algae is the highest, and the lowest in winter months. It should be noted that during the second scenario (the selected area for year-round raw materials such as algae, can be different each month) all the available area for algae is used in

January and February, whilst in July when the algal yield is the highest, only around 19 % of the available area for algae is used. The reason for much higher storage capacity during the second scenario is that production in summer months is much higher than in winter months, however all the produced algae has to be used for biodiesel production.

Since the profit is much higher for those cases when not all of the available year-round raw materials are used for bioenergy, in the next scenarios (third – fifth scenario) the selected area could be different for each month. Seasonal raw materials (corn and wheat), switchgrass and forest residue could be harvested over optimal time period(s).

4.2.3.3 Third Scenario

During the third scenario, it is assumed that the cultivation area for biomass devoted to biofuels could not exceed a specific percentage of the land area in each zone. The cultivation area from up to 2 % to up to 20 % of the total area is assumed, with step-sizes of 2 %. The flowrates of raw materials are shown in Figure 4-12, the flowrates of products in Figure 4-13, and the profit in Figure 4-14 for those specific percentages of the land area devoted to biofuels.

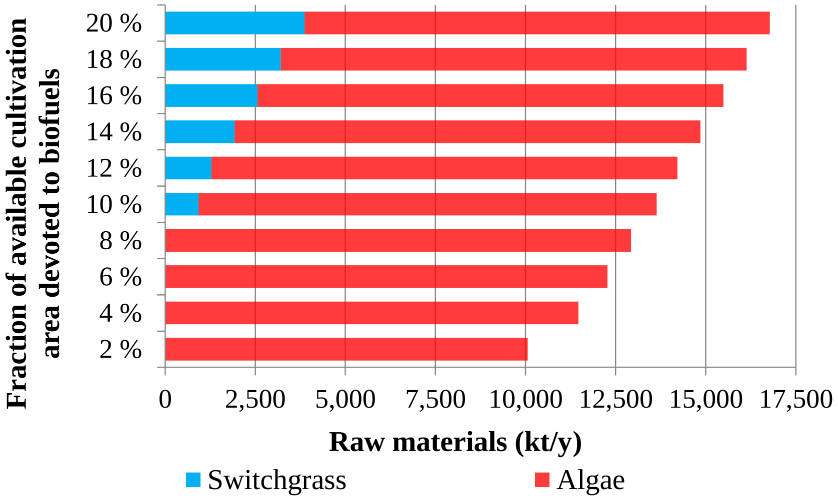


Figure 4-12. The consumption of raw materials in regard to different fractions of cultivation area devoted to biofuels (Čuček et al., 2013c)

From Figure 4-12 it can be seen that the most profitable raw material is algae, mainly due to the higher yield to fuels, whilst when capacities of plants converting algae to biofuels are reached, also switchgrass is used for biofuels production. Using up to 2 % of the cultivation area the capacities of biodiesel production plants are almost reached, and therefore when increasing the fraction of cultivated area, the consumption of algae is not proportional. At available 2 % of cultivation area, almost all the available area during the year is cultivated for algae, whilst for higher percentages, more area is used in winter months when the algal yield is lower, and less area in especially summer when the algal yield is higher. The most profitable technology is transesterification of algal oil using methanol. The capacities of biodiesel production plants are finally reached by 10 % of the available area devoted to biofuels, when also switchgrass is consumed for biofuels. The most profitable technology converting switchgrass to biofuels is gasification and further syngas fermentation, where ethanol and small amount of hydrogen are produced.

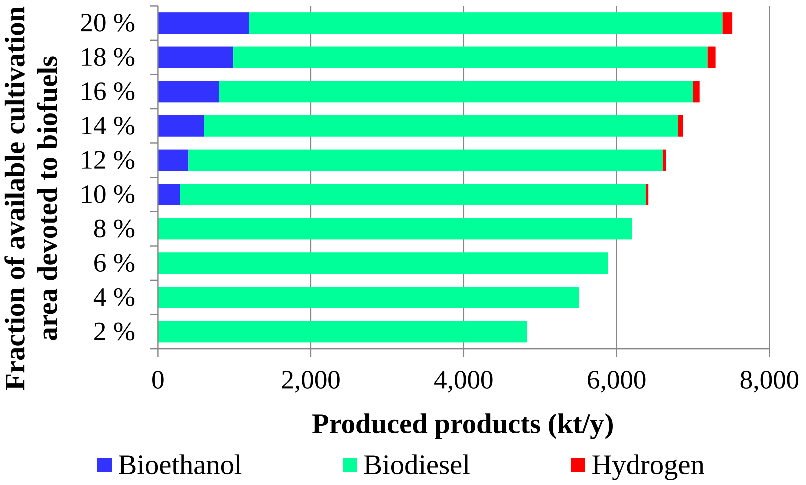


Figure 4-13. The production of biofuels in regard to different fractions of cultivation area devoted to biofuels (Čuček et al., 2013c)

Figure 4-13 shows the production of biofuels (bioethanol, biodiesel and hydrogen) when a certain percentage of cultivation area is devoted to it. Similar trend as from Figure 4-12 can be seen, since algae are used for biodiesel, whilst switchgrass is for bioethanol and hydrogen production. Since algae are converted to biodiesel, similarly only biodiesel is produced till 10 % of the area. From the 10 % of the area upwards, bioethanol and hydrogen are also produced from switchgrass.

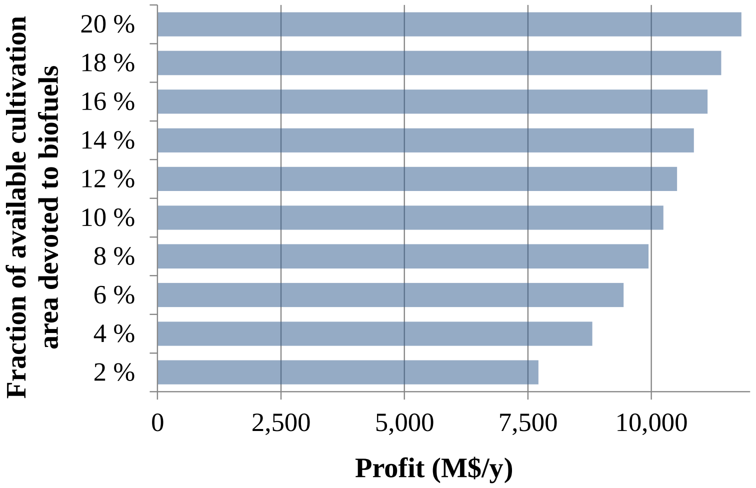


Figure 4-14. The profit in regard to different fractions of cultivation area devoted to biofuels (Čuček et al., 2013c)

Again, a similar trend is shown from Figure 4-14 as from Figure 4-12 and Figure 4-13. The profit is already significant when using only up to 2 % of the cultivation area due to algae consumption and biodiesel production. The profit further gradually increases; however, steeper for the lower fractions of cultivation area devoted to biofuels. When devoting up to 20 % of area to biofuels, the profit is higher by only around 50 % compared to the case when using only 2 % of the area (11,825 M$/y vs. 7,713 M$/y), especially due to higher algae yield and expensive technology of second-generation bioethanol production.

4.2.3.4 Fourth Scenario

It is assumed during the fourth scenario that the cultivation of food-crops would also have to be done within the available cultivation area in order to prevent competition between fuels and food production. Of the total harvesting area it is considered that the corn and/or wheat grain uses from 0 % up to 20 % with step-sizes of 2 % to evaluate the effect on the profitability. The produced grains are direct products and used only for food; their residues, however, could be utilised for biofuels. The remaining harvesting area not intended for food (up to 20 % of the total area of each zone) can be used for biofuels production.

The flowrates of the raw materials are shown in Figure 4-15, the flowrates of the products in Figure 4-16, and the profit in Figure 4-17 for those different sections of the cultivated area used for food-crops.

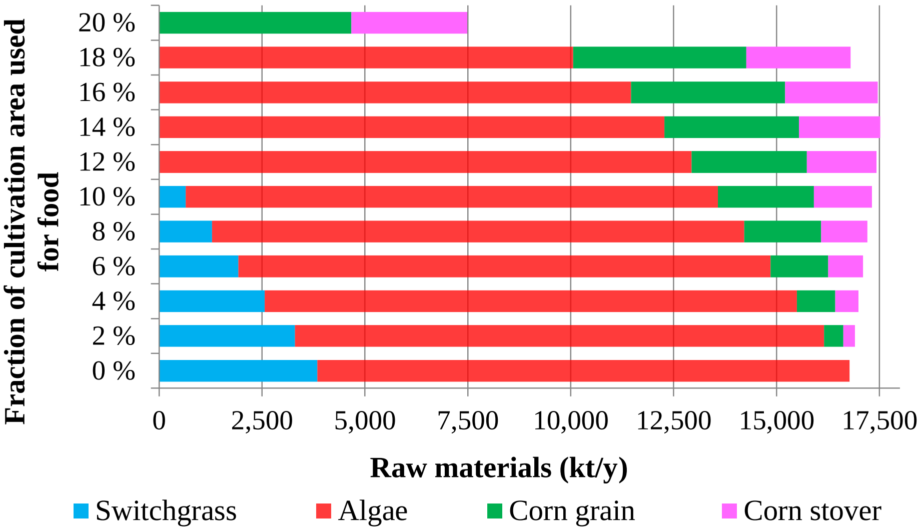


Figure 4-15. The consumption of raw materials from the different sections of those areas used for food crops (Čuček et al., 2013c)

It can be seen from Figure 4-15 that by increasing the percentage of cultivated area for food-crops, less switchgrass is cultivated, whilst more corn grain and stover are produced. It can be seen that from amongst the different types of grain, corn is an economically more preferable crop. Algae are the most economically-profitable crop, and are produced in all cases except when all the available area for fuels and food is intended for food-crops.

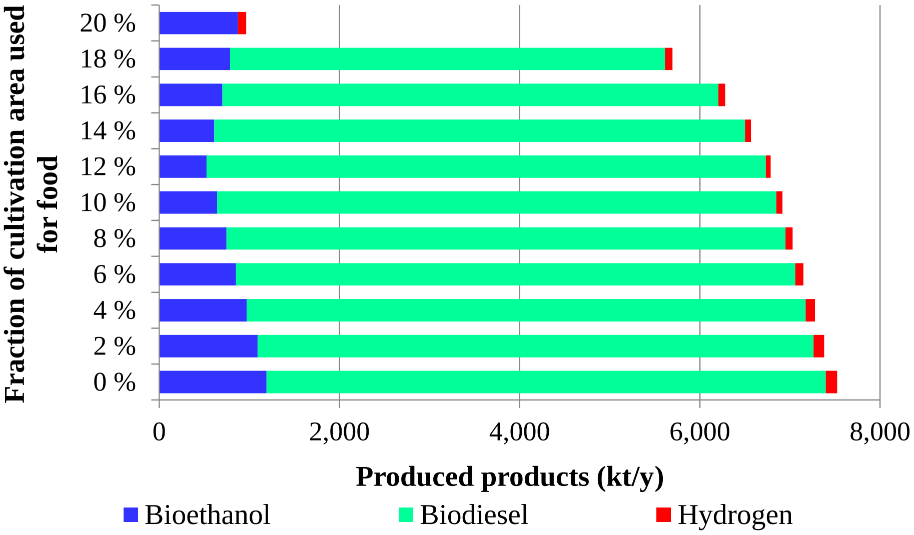


Figure 4-16. The production of biofuels from the different sections of those areas used for food crops (Čuček et al., 2013c)

It can be seen from Figure 4-16 that most of the produced biofuels corresponds to biodiesel, which is produced from algal oil. Algae have a much higher yield compared to all the other raw materials (18,250 t/(km^{2}y) vs. 1,000 t/(km^{2}y) for switchgrass that has the second-best yield). The production rate of ethanol and hydrogen decreases by lower fractions of area intended for food-crops, since less switchgrass is used for biofuels, whilst at higher fractions it increases again due to a higher consumption of corn stover. The lowest ethanol and hydrogen yields are by those fractions of available cultivation area used for biofuels and food, when switchgrass is no longer produced (by 12 %).

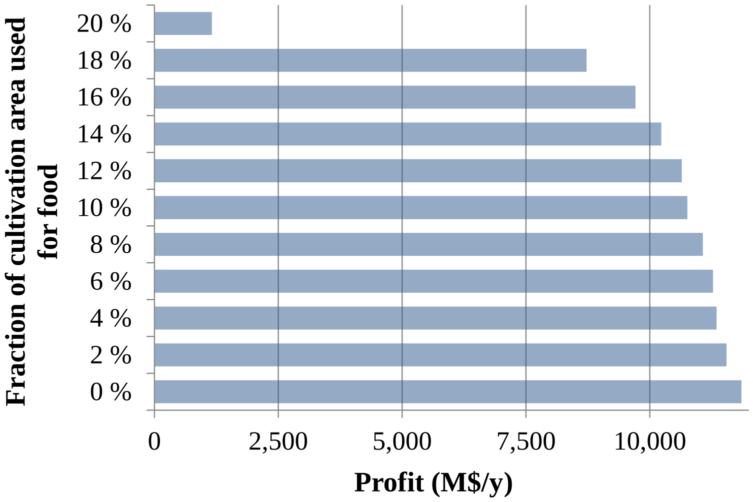


Figure 4-17. Profits from the different sections of those areas used for food crops (Čuček et al., 2013c)

Profit is the highest when none of the crops are being used food-crops, whilst much lower when the entire cultivated area is intended for food-crops, and their residues for biofuels (bioethanol and hydrogen), see Figure 4-17. This is where the ethical problem begins. From an economic point of view it is more interesting to produce fuels but food is needed to feed the population. Significant difference in profit can be seen from Figure 4-17 when increasing the cultivation area for corn and wheat plants from 18 to 20 % (8,724 M$/y vs. 1,159 M$/y), since the most profitable biomass, algae, is not produced. Due to a high algal yield, the profit is significantly reduced when algae are no longer produced. At around 2 % of the cultivation area, already more than 65 % of the capacities for biodiesel production are already reached. It should be noted that the profit by 0 % of the cultivation area used for food equals the maximal profit obtained when 20 % of the available cultivation area is devoted to biofuels (see Figure 4-14).

4.2.3.5 Fifth Scenario

It is assumed during the fifth scenario that the demand for biofuels (bioethanol and biodiesel) and food (corn and wheat grain) should be satisfied. The demand for corn within the region is 387.71 kt/y, and the demand for wheat 308.35 kt/y (Cummans, 2012). The demand for biofuels should be 20, 50 and 100 % of gasoline and diesel consumption within the region. Three different demand patterns are assumed, world, EU and US average road sector for diesel (The World Bank, 2013a) and gasoline fuel consumption (The World Bank, 2013b). The fuel consumptions per capita for the three patterns are shown in Table 4-10.

It should be noted that bioethanol and green diesel (sum of biodiesel and FT-diesel, where for simplicity the calorific value of 40 MJ/kg is considered for both green diesels) consumption is calculated in regard to the calorific values of gasoline and diesel (47.3 MJ/kg and 44.8 MJ/kg). For the reasons of simplification it is assumed that other biofuels, such as hydrogen and green gasoline, as well as utilities are entirely demanded if they are produced. During this scenario it is assumed that, except for the case of the US demand pattern, up to 20 % of the total area of each zone could be dedicated to biofuels and food. In order to satisfy the demand for ethanol, up to 60 % of the each zone total area is assumed when applying the demand pattern of the US.

Table 4-10. Road sector gasoline and diesel fuel consumption per capita

Fuel	World	EU	US
Gasoline (kg/(capita·y))	127	164	1,047
Diesel (kg/(capita·y))	124	373	392

Four additional Equations are added within the model to account for demand for bioethanol – Equation (4.66), biodiesel – Equation (4.67), corn grain – Equation (4.68), and wheat – Equation (4.69) within the region:

$$Dem_{\text{bioethanol}} = \sum_{n\in N}\sum_{t\in T}\sum_{j\in J}\sum_{tp\in TP} q_{n,t,j,\text{bioethanol},tp}^{m,\text{T,L3,L4}} \tag{4.66}$$

$$Dem_{\text{biodiesel}} = \sum_{n\in N}\sum_{t\in T}\sum_{j\in J}\sum_{tp\in TP} q_{n,t,j,\text{biodiesel},tp}^{m,\text{T,L3,L4}} \tag{4.67}$$

$$Dem_{\text{corn grain}} = \sum_{m\in M}\sum_{j\in J}\sum_{tp\in TP} q_{m,j,\text{corn grain},tp}^{m,\text{L2,L4}} \tag{4.68}$$

$$Dem_{\text{wheat}} = \sum_{m\in M}\sum_{j\in J}\sum_{tp\in TP} q_{m,j,\text{wheat},tp}^{m,\text{L2,L4}} \tag{4.69}$$

In all the cases regarding demand patterns, the demand for transportation fuels could be satisfied entirely (100 % of gasoline and diesel consumption within the region) by biofuels (bioethanol and biodiesel). In the case of the EU and world average demand patterns, the demand for food and transportation fuels could be reached by using up to 20 % of the total region’s area, whilst in the case of US average demand patterns, the demand for food and transportation fuels could also be reached, but by using up to 60 % of the total region’s area in order to satisfy the demand for ethanol. The reason for larger land area requirement in the case of US average demand patterns lay in high bioethanol consumption, due to high gasoline consumption per capita (see Table 4-10). The main results when satisfying the demand for food (corn and wheat) and fuels (bioethanol and biodiesel) for all the demand patterns (world, EU, and US averages) are shown in Figure 4-18 – Figure 4-20. The profits are shown in Figure 4-18, the consumption of raw materials in Figure 4-19, and the production of direct (food) and produced products (biofuels) in Figure 4-20.

It can be seen that the profits are the lowest when accounting for the world average energy consumption, and the highest when accounting for the US average energy consumption. US energy consumption is, on average, the highest and the world average energy consumption, on average, the lowest from amongst those selected demand patterns. When increasing the demand for biofuels from 20 – 100 % the profit is also increased, which means that production of bioethanol and biodiesel is more profitable than the production of other biofuels such as hydrogen. Hydrogen and also green gasoline can be produced within the region, and for them the demand is unspecified. Namely, when all the demanded food and fuels are satisfied, the production of hydrogen is only limited to the maximal area available for food and fuel production. When accounting for the world and EU average energy consumptions, up to 20 % of the total area would suffice, whilst when accounting for the US average energy consumption, the total region’s area would need to be increased to 60 % in order to satisfy the demand for bioethanol.

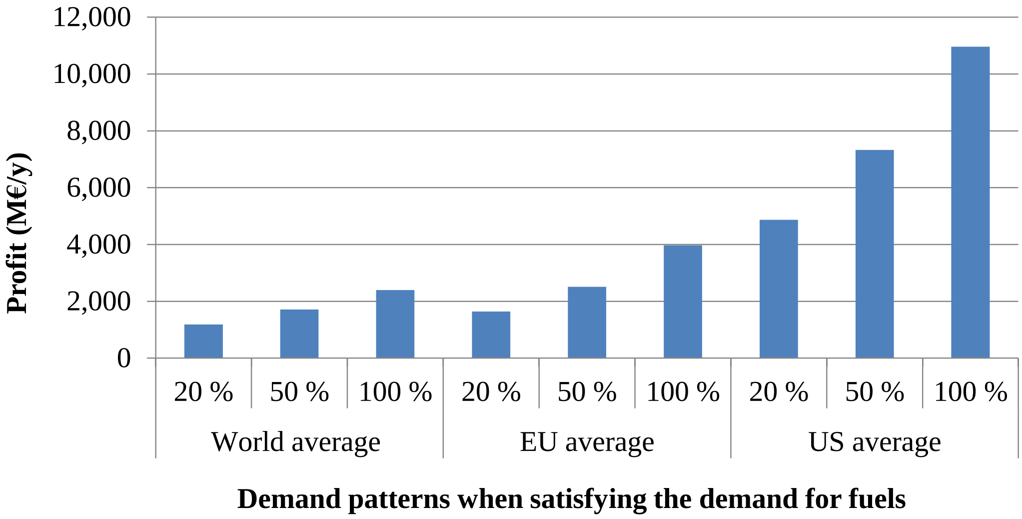


Figure 4-18. Profits when satisfying the demand for food and fuels (Čuček et al., 2013c)

Those results show that on the world's level, as well as within the EU, the demand for food can be satisfied, as well as petroleum fuels can be entirely replaced by biofuels when using 20 % of the total area. However, it should be noted, that regional characteristics should be considered, such as solar irradiance, air temperature, presence of mountains, leaks, and deserts etc., where biomass cannot be grown or its growth is limited.

Figure 4-19 shows the consumption of raw materials when satisfying the demand for food and fuels, where the consumption of switchgrass is due to its size reduced by factor of ten to fit Figure 4-19.

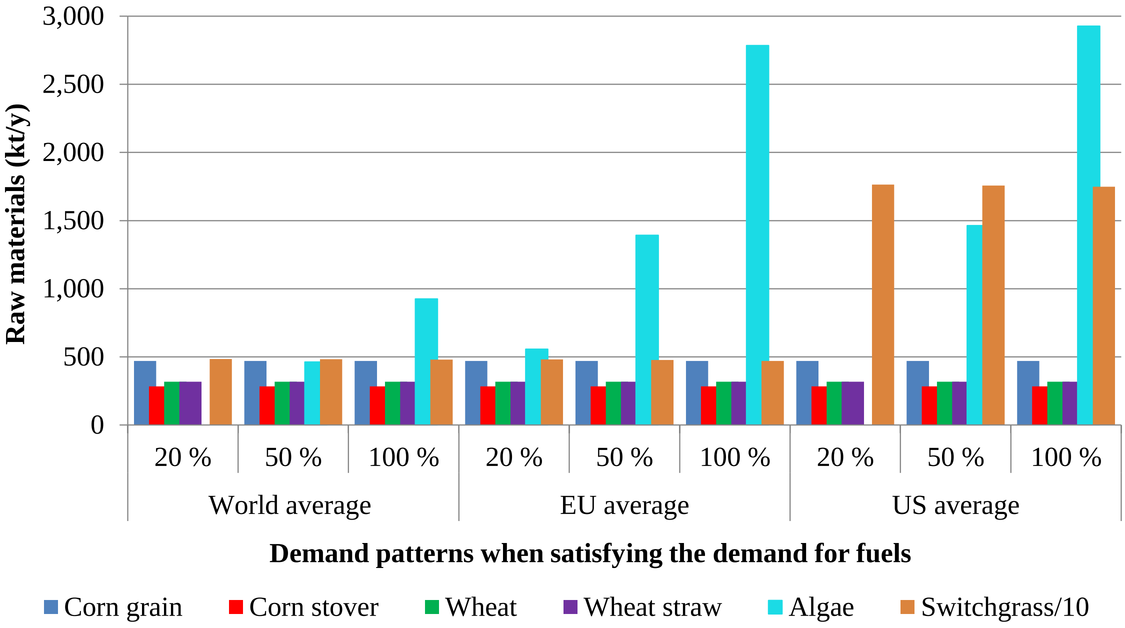


Figure 4-19. Raw materials consumption when satisfying the demand for food and fuels (Čuček et al., 2013c)

It can be seen from Figure 4-19 that corn grain and wheat production is the same for all the different demand patterns for fuels. It is namely assumed that the demand for food should be satisfied, and that this demand is also the same for all the cases. Corn and wheat residues are used at their maximum available capacity. The main biomass sources for bioenergy production are switchgrass and algae. Switchgrass is used to satisfy the demand for bioethanol and part of biodiesel, whilst algae to satisfy the demand for biodiesel.

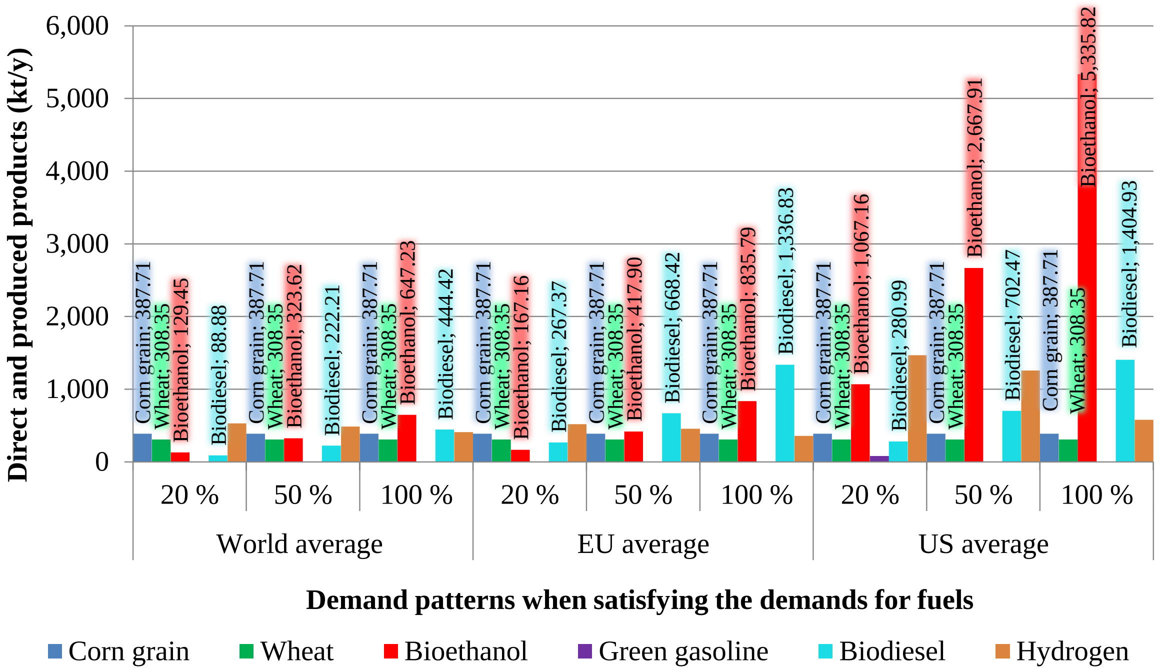


Figure 4-20. The production of products when satisfying the demand for food and fuels (Čuček et al., 2013c)

It can be seen from Figure 4-20 that the demand for food and biofuels is satisfied. Besides the demanded products, hydrogen could also be produced for which the demand is unspecified. It should be noted that when all the demands for food and fuels are satisfied, the production of hydrogen is limited only to the maximal area available for food and fuel production. Therefore, the production of hydrogen is the highest when the demand for biofuels is 20 %, and the lowest when the demand for biofuels is 100 % of the average transportation fuel consumption. The optimal technologies selected are gasification and syngas fermentation, transesterification of algal oil with methanol, FT-diesel and green gasoline production, and hydrogen production.

5 ASSESSMENT METHODS FOR SUSTAINABLE DEVELOPMENT WITHIN MULTI-OBJECTIVE OPTIMISATION

This Chapter is divided into three parts. All three parts deal with MOO approaches when considering direct, indirect, and total (direct and indirect) effects on the environment. Different environmental (sustainability) metrics are proposed for supporting environmental (sustainability) assessments. The first part deals with direct, indirect, and total footprints (Čuček et al., 2012e), the second part with direct, indirect, and total sustainability indexes (Kravanja and Čuček, 2013), and the last part with eco-cost, eco-benefit, eco-profit (Čuček et al., 2012a), net profit, and total profit (Kravanja and Čuček, 2013).

The selection and accuracy of the data are essential for ensuring an accurate and reliable analysis of the systems impacts on the sustainability and SD. In this way sustainable solutions are defined as well as critical activities ("hot spots"). However, it should be noted that environmentally-related data vary significantly in the literature, whilst social impacts are usually overlooked. Environmental impacts are namely specific for any system regarding location, time, technology, and composition, to name but a few. Therefore, proper evaluation of sustainability and SD without measuring these impacts is impossible. These presented cases in this Section are just illustrative examples. However, the assessment methods and methodologies presented can be applied to any other system.

5.1 Footprints

A "footprint" is a quantitative measurement describing the appropriation of natural resources by humans (Hoekstra, 2008). A footprint describes how human activities can impose different types of burdens and impacts on global sustainability (UNEP/SETAC, 2009).

It should be noted that footprints are usually considered as being measured in units of area. However, the data expressed in area units show high variability and highly possible errors regarding the results. The conversion into a land area would have to be based on a variety of different assumptions and would increase those uncertainties and errors associated with a particular footprint estimate – see e.g. (Wiedmann and Minx, 2008). Converting some of the footprints into area units can prove to be problematic, especially for processes that are not primarily area-based, such as chemical processes (De Benedetto and Klemeš, 2009). Ecological footprint and its categories, the SPI, and the SEPI are always defined in units of area, however footprints other than these, are not usually defined (only) in area units (Čuček et al., 2012c).

Several environmental footprints are considered, such as CF, energy (EF), water (WF), water pollution (WPF) and land (LF) footprints. In addition to these, a food-to-energy footprint (FEF) is defined in order to evaluate the risk of diverting farmland for the production of fuel rather than food.

CF stands for a certain amount of gaseous emissions relevant to climate change, and is associated with human production and consumption activities (Wiedmann and Minx, 2008). Although the "climate footprint" (Wiedmann and Minx, 2008) and "GHG footprint" are more appropriate, the term "carbon footprint" is used, mainly due to its broader acceptance so far. CF is usually defined based on the amount of CO_2 and other GHGs emitted over the full life-cycle of a product, process or activity, and expressed in mass unit per functional unit (UK Parliamentary Office of Science and Technology (POST), 2011).

Various definitions of an EF have been defined. One of its definitions is that it represents the demand for non-renewable energy resources (Schindler, 2013). EF is expressed in energy unit per functional unit.

WF is closely linked to the concept of virtual water and represents the total volume of direct and indirect fresh water used, consumed and/or polluted (Hoekstra, 2003). WF consists of blue, green, and grey water footprints that represent the consumption of surface and ground water, the consumption of rainwater, and the volume of water required to dilute pollutants to water quality standards (Mekonnen and Hoekstra, 2010). WF is expressed in volume unit per functional unit.

LF stands for the agricultural land area used for growing biomass for both food and energy (Kissinger and Gottlieb, 2010), expressed in area unit per functional unit.

WPF stands for the amount of substances emitted into water within the environment, expressed in mass unit per functional unit (Sánchez-Chóliz and Duarte, 2005).

FEF is defined as a mass flow rate of energy converted from food-intended crops, expressed in mass unit per functional unit (Čuček and Kravanja, 2010).

5.1.1 Direct, Indirect and Total Footprints

The aim of this research work is the development of regional supply chains that would include various environmental and social footprints, based on direct, indirect, and total footprints (the sum of direct and indirect footprints) along the whole supply chain.

Direct environmental footprints, and any sustainability metric, conventionally measure only direct harmful effects (burdens) on the environment. Direct footprints are related to the extraction of resources, materials' production, usage, maintenance, recycling and/or disposal, including all transportation and distribution steps. However, when a system, in addition to its direct burdening effects on the environment, exhibits a significant unburdening effect on the environment, by considering only direct effects, may result in misleading solutions.

Indirect footprints represent an unburdening of the environment by harmful products' substitution with benign products, and the utilising of harmful products rather than discarding them. Several examples include when waste is utilised instead of being discarded, when environmentally-benign raw materials, products and services are used instead of harmful ones, or when conventional energy is replaced by biomass energy; and the indirect effect is a reduction in the footprint. Indirect footprints indirectly unburden or benefit the environment.

Total footprints are defined as a sum of direct and indirect footprints. Considering total effects enables the obtaining of more realistic solutions than in those cases when only direct effects are considered. An appropriate sustainable synthesis should identify those solutions that unburden the environment the most, rather than only proposing the least-burdening solutions.

5.1.2 Implementation of Footprints' Evaluations within Supply Chains

Mathematical model of regional supply chains (see Section 4.1 and (Lam, 2010)) is extended to employ various direct, indirect, and total footprints along the whole supply chain. Different environmental and social footprints are taken into consideration. As a result, the mathematical model employs various direct, indirect, and total footprints along the whole supply chain. Footprints are defined as per year and per unit of the supply-chain network's total area (A, km^2).

The model is formulated in the MINLP form. The following additional sets are defined within the model (Equations (5.1) – (5.9)):

i) Set PS for substituted products with elements $ps \in PS$.

ii) Set FP for environmental and social footprints with elements $f \in FP$.

iii) Set $PSP = PS \times PP$ for pairs of substituted product and produced product (if a produced product substitutes conventional product) with elements $(ps, pp) \in PSP$.

5.1.2.1 *Direct Environmental Footprint*

For the supply layer, direct environmental footprint type $f \in FP$, F_f^{L1}, is calculated from the production rate $q_{i,pi}^{m,\mathrm{L1}}$ of biomass type pi within the supply zone i, multiplied by the specific environmental footprint $ei_{f,pi}^{\mathrm{L1}}$, caused by growing the biomass, divided by the supply network's total area (A):

$$F_f^{\mathrm{L1}} = (\sum_{i\in I}\sum_{pi\in PI} q_{i,pi}^{m,\mathrm{L1}} \cdot ei_{f,pi}^{\mathrm{L1}})/A \qquad \forall f \in FP \tag{5.1}$$

For the pre-treatment layer, F_f^{L2} is defined as the mass-flow rate of biomass pi from the supply zone i in L1 to the pre-treatment centre m in L2, multiplied by the specific environmental footprint for that biomass, $ei_{f,pi}^{\mathrm{L2}}$, caused by pre-processing, and also evaluated per unit of total area:

$$F_f^{\mathrm{L2}} = (\sum_{i\in I}\sum_{m\in M}\sum_{pi\in PI} q_{i,m,pi}^{m,\mathrm{L1,L2}} \cdot ei_{f,pi}^{\mathrm{L2}})/A \qquad \forall f \in FP \tag{5.2}$$

For the processing layer, F_f^{L3} is obtained as the mass-flow rate of the intermediate product pi to the selected technology t at process plant n in L3, multiplied by the specific environmental footprint for that product, $ei_{f,pi,t}^{\mathrm{L3}}$, caused by processing and divided by the network's total area:

$$F_f^{\mathrm{L3}} = (\sum_{n\in N}\sum_{(pi,t)\in PIT} q_{n,pi,t}^{m,\mathrm{T,L3}} \cdot ei_{f,pi,t}^{\mathrm{L3}}))/A \qquad \forall f \in FP \tag{5.3}$$

For the use layer, F_f^{L4} is calculated as the mass flowrate of the directly-used products pd from L2 (see Figure 4-1), and produced products pp from L3 ($q_{m,j,pd}^{m,\mathrm{L2,L4}}$ and $q_{n,j,pp}^{m,\mathrm{L3,L4}}$), each multiplied by the specific environmental footprint for this product, $ei_{f,pd}^{\mathrm{L4}}$ and $ei_{f,pp}^{\mathrm{L4}}$, caused by their usage and divided by the network's total area:

$$F_f^{\mathrm{L4}} = (\sum_{m\in M}\sum_{j\in J}\sum_{pd\in PD} q_{m,j,pd}^{m,\mathrm{L2,L4}} \cdot ei_{f,pd}^{\mathrm{L4}} + \sum_{n\in N}\sum_{j\in J}\sum_{pp\in PP} q_{n,j,pp}^{m,\mathrm{L3,L4}} \cdot ei_{f,pp}^{\mathrm{L4}})/A \qquad \forall f \in FP \tag{5.4}$$

Finally, for the transportation of materials between layers, the environmental footprint F_f^{tr} is also defined per the network's total area. Its value depends on the density of the biomass, distances $(D_{x,y}^{\mathrm{L}a,\mathrm{L}b})$, mode of transport, rate of biomass supply $(q_{x,y,p}^{m,\mathrm{L}a,\mathrm{L}b})$ and road conditions $(f_{x,y}^{\mathrm{road},\mathrm{L}a,\mathrm{L}b})$. The specific environmental footprint $(ei_{f,p}^{\mathrm{tr},\mathrm{L}a,\mathrm{L}b})$ is defined per t·km:

$$\begin{aligned} F_f^{\mathrm{tr}} = (&\sum_{i\in I}\sum_{m\in M}\sum_{pi\in PI} D_{i,m}^{\mathrm{L1,L2}} \cdot f_{i,m}^{\mathrm{road,L1,L2}} \cdot ei_{f,pi}^{\mathrm{tr,L1,L2}} \cdot q_{i,m,pi}^{m,\mathrm{L1,L2}} + \\ &\sum_{m\in M}\sum_{n\in N}\sum_{pi\in PI} D_{m,n}^{\mathrm{L2,L3}} \cdot f_{m,n}^{\mathrm{road,L2,L3}} \cdot ei_{f,pi}^{\mathrm{tr,L2,L3}} \cdot q_{m,n,pi}^{m,\mathrm{L2,L3}} + \\ &\sum_{m\in M}\sum_{j\in J}\sum_{pd\in PD} D_{m,j}^{\mathrm{L2,L4}} \cdot f_{m,j}^{\mathrm{road,L2,L4}} \cdot ei_{f,pd}^{\mathrm{tr,L2,L4}} \cdot q_{m,j,pd}^{m,\mathrm{L2,L4}} + \\ &\sum_{n\in N}\sum_{j\in J}\sum_{pp\in PP} D_{n,j}^{\mathrm{L3,L4}} \cdot f_{n,j}^{\mathrm{road,L3,L4}} \cdot ei_{f,pp}^{\mathrm{tr,L3,L4}} \cdot q_{n,j,pp}^{m,\mathrm{L3,L4}})/A \qquad \forall f \in FP \end{aligned} \tag{5.5}$$

Equation (5.5) represents the environmental footprint caused by transporting biomass pi from L1 to L2 (the first term), intermediate product pi from L2 to L3 (the second term), the directly-used product pd from L2 to L4 (the third term), and the produced products pp from L3 to L4 (the last term).

5.1.2.2 Indirect Environmental Footprint

The indirect environmental footprint F_f^{ind}, for the use of biomass is defined as the unburdening related to the utilising of harmful products, and the substitution of conventional, mainly non-renewable products. The correlation between conventional energy and biomass energy is defined by the substitution factor $f_{ps,pp}^{\mathrm{sub}}$, where $ps \in PS$ is the substituted product. With the generation of bioenergy and bioproducts, the supply and consumption of previously-used resources is reduced by the amount specified by the substitution factors.

F_f^{ind} is defined as the product between the specific environmental footprint for the substituted product $ei_{f,ps}^{\mathrm{sub}}$, the substitution factor for that product $f_{ps,pp}^{\mathrm{sub}}$, and the mass-flow of the biomass product converted in the plant $q_{n,j,pp}^{m,\mathrm{L3,L4}}$, per unit of total area.

$$F_f^{\mathrm{ind}} = -\Big(\sum_{(ps,pp)\in PSP} ei_{f,ps}^{\mathrm{sub}} \cdot f_{ps,pp}^{\mathrm{sub}} \cdot \sum_{n\in N}\sum_{j\in J}\sum_{pp\in PP} q_{n,j,pp}^{m,\mathrm{L3,L4}}\Big)/A \qquad \forall f \in FP \tag{5.6}$$

Note that the F_f^{ind} is negative, as the substitution causes unburdening.

5.1.2.3 Total Environmental Footprint

The total environmental footprint of the supply chain's network (F_f) is defined as a summation of all the direct footprint elements, and the indirect footprint correction:

$$F_f = F_f^{\mathrm{L1}} + F_f^{\mathrm{L2}} + F_f^{\mathrm{L3}} + F_f^{\mathrm{L4}} + F_f^{\mathrm{tr}} + F_f^{\mathrm{ind}} \tag{5.7}$$

5.1.2.4 Food-to-Energy Footprint

FEF is included for two reasons, because of food vs. fuel competition and any related possible increase of food prices. Food vs. fuel competition for biomass utilisation is a very important issue relating to the usage of biomass for fuels (first generation biofuels) that needs to be considered. This problem is emphasised by the Nestlé chief executive: "*If, as predicted, we look to use biofuels to satisfy 20 % of the growing demand for oil products, there will be nothing left to eat*." (Asch and Heuelsebusch, 2009). Another problem relating to the biofuel industry is the global increase of food prices (IndexMundi, 2013) that may be the result of using more crops and land for energy purposes.

FEF is only defined for those multi-functional (multi-product) crops that can result in a supply of food, feed, and energy. Biomass crops, which may take land that could be used for growing food crops, are unconsidered in this footprint (FEF is zero). This social footprint is defined as a mass flowrate for pairs of food-crop products and the applicable process technology for them ($q_{n,pi,pp,t}^{m,\mathrm{T,L2,L3}}$), divided by the weight loss by drying, the conversion of intermediates into products ($f_{pi}^{\mathrm{conv,L2}}$), and the mass flowrate of food-intended crops ($q_{i,m,pi}^{m,\mathrm{L1,L2}}$) excluding water ($w_{\mathrm{H_2O}}$). The FEF is divided by the network's total area:

$$\mathrm{FEF} = \left(\frac{\sum\limits_{n \in N} \sum\limits_{(pi,pp) \in PIPP} q_{n,pi,pp,t}^{m,\mathrm{T,L2,L3}}}{f_{pi}^{\mathrm{conv,L2}} \cdot \left(\sum\limits_{i \in I} \sum\limits_{m \in M} \sum\limits_{pi \in PI} q_{i,m,pi}^{m,\mathrm{L1,L2}} \cdot (1 - w_{\mathrm{H_2O}}) \right)} \right) / A \qquad (5.8)$$

5.1.2.5 Two-Step Multi-Criteria Approach

The synthesis of biomass energy supply chain networks when considering direct, indirect and total footprints is performed over two steps. During the first MINLP step (MINLP-1) the synthesis model is solved with the objective of maximising profit. Firstly, MINLP-1 is used to obtain an initial or reference solution, representing the maximum profit possible / upper bound of the profit. This is then followed by solving the second MINLP step (MINLP-2) for obtaining the multi-objective optimal solution(s).

MOO is performed at MINLP-2 by applying the ε-constraint method for each iteration k, $k \in K$. A sequence of constrained single-objective $(\mathrm{MINLP}-2)_{f,k}$ problems is solved for each footprint f, as the maximisation of the profit P subjected to a relative footprint $(F_{f,k}^{r})$. The relative footprint is defined as the footprint obtained at MINLP-2 $(F_{f,k}(x))$ divided by the footprint obtained at MINLP-1 $(F_{f}^{0}(x))$. It decreases sequentially from the maximal footprint obtained at MINLP-1 by a suitable step-size until there is no feasible solution.

The synthesis problem at MINLP-2 takes the following form:

$$
\begin{aligned}
&\max_{x,y}\; P_k = c^{\mathrm{T}} y + f(x) - \sum_{f \in FP} w \cdot F_f(x) \\
&\text{s.t.} \quad Ay + h(x,y) = 0 \\
&\qquad\;\; By + g(x,y) \le 0 \\
&\qquad\;\; F^{r}_{f,k}(x) \le \varepsilon_k \\
&\qquad\;\; (x^{\mathrm{LO}} \le x \le x^{\mathrm{UP}}) \in X \subset R^n, \;\; y \in Y = \{0,1\}^m \\
&\qquad\;\; \varepsilon_{k-1} = \varepsilon_k - \Delta\varepsilon, \;\; \Delta\varepsilon = \frac{1}{N}, \;\; \varepsilon_1 = 1, \;\; k \in K = \{1, \ldots, N+1\}
\end{aligned}
\qquad (\mathrm{MINLP}-2)_{f,k}, \forall f \in FP
$$

where relative footprint $(F^{r}_{f,k}(x))$ is defined as:

$$
F^{r}_{f,k}(x) = \frac{F_{f,k}(x)}{F^{0}_{f}(x)} \tag{5.9}
$$

$(\mathrm{MINLP}-2)_{f,k}$ is performed separately for each footprint *f*. Footprints are also minimised with a small weight *w* to provide solutions with the least values for those footprints in those cases where multiple footprint solutions exist. The weight should be very small in order not to interfere with the maximisation of profit, e.g. 10^{-6}.

At MINLP-2 two sets of MOOs are performed, maximising the profit whilst simultaneously minimising i) the relative direct footprints, and ii) the relative total footprints. Different sets of Pareto optimal solutions, one for each footprint, are generated at MINLP-2 as 2-D projections of a multi-D problem, and so the subjective aggregation of different footprints, since they are usually expressed in different units, is thus avoided.

Note that in the case of negative footprints, ε-inequality constraint is changed into an equality constraint and a SOO is performed. In this way, non-trade-off optimal solutions are obtained by the sequence of $(\mathrm{MINLP}-2)_{f,k}$ where profit is maximised whilst relative footprints are incrementally increased from -1 to zero of even some positive values until there is no feasible solution at zero profit.

5.1.3 Illustrative Example

The above presented concept and developed model is applied within a regional biomass and bioenergy supply network – the model and illustrative example (Lam, 2010). The integrated MINLP model consists of around 1,100 continuous variables, 20 binary variables, and 650 constraints and could be solved in a fraction of second using DICOPT/GAMS on a computer with 2.33 GHz Intel® Core™2 Quad Q8200 processor with 4.00 GB of RAM.

5.1.3.1 Direct Footprints

The data for the raw materials' various direct specific environmental footprints are given in Table 5-1. Specific environmental footprints are defined in t (WF, WPF and CF), and in GJ (EF) per t of biomass.

Table 5-1. Direct specific environmental footprints for biomass

	Water (t/t)	Non-renewable energy consumption (GJ/t)	Emissions to water (t/t)	Emissions to air (t/t)
Corn grains	900	1.73	0.032	0.154
Corn stover**	900	1.73	0.032	0.154
Organic manure	0.75*	-	-	-
Wood chips***	2,500	0.75	-	0.066
MSW	0.229*	-	-	-
Timber	1,500	0.5	-	0.044

*Since organic manure and MSW are waste, there is no available data on WF, and only raw materials moisture is taken as WF

**Assuming that from the entire plant mass around 50 % is grain and 50 % stover (Čuček et al., 2011b)

***Assuming the density of wood chips is approximately half density of timber (Čuček et al., 2010)

The data for various direct specific footprints caused by pre-treatment and processing per t of intermediate product are given in Table 5-2.

Table 5-2. Direct specific environmental footprints for pre-treatment and processing

	Water (t/t)	Non-renewable energy consumption (GJ/ t)	Emissions to water (t/t)	Emissions to air (t/t)
Dry-grind process	1.3	2.5	-	0.147
MSW incineration	0.31*	-	0.0016	0.415
AD	0.091	-	-	-
Sawing	10.6	0.036	-	0.00125
Corn stover compressing	0.005	0.01504	-	0.00262
Corn grain drying	0.5	1.251	-	0.09
Timber drying	0.004	0.0108**	-	0.00078

*a little higher WF than moisture content of MSW is assumed, 22.9 % (Čuček et al., 2010))

**air and kiln drying of wood is assumed where thermal energy for kiln drying is obtained from wood

Table 5-3 presents the direct specific environmental footprints for transport (in t/(t·km) and in GJ/(t·km)). Biomass is assumed to be transported by truck from L1 to L2 with consumption of 0.3 L of petrol/km. Intermediate products are transported by rail from L2 to L3. Transport of direct products (corn intended for food) to consumers is assumed to be partly by truck, partly by rail, and produced products to consumers by truck. Bioethanol is transported to filling stations by tank trailers (cisterns). Electricity is distributed by alternating current power lines; and heat is used for buildings and water heating.

Table 5-3. Direct specific environmental footprints for transport

	Water (t/(t·km))		Non-renewable energy consumption (GJ/(t·km))*		Emissions to water (t/(t·km))		Emissions to air (t/(t·km))	
	Road	Rail	Road	Rail	Road	Rail	Road	Rail
Corn grains	$1.36\cdot10^{-4}$	$7.3\cdot10^{-5}$	$3.89\cdot10^{-4}$	$2.08\cdot10^{-4}$	-	-	$5.3\cdot10^{-5}$	$8\cdot10^{-6}$
Corn stover	$2.33\cdot10^{-3}$	$1.25\cdot10^{-3}$	$6.67\cdot10^{-3}$	$3.57\cdot10^{-3}$	-	-	$1.1\cdot10^{-3}$	$8\cdot10^{-6}$
Manure, digestate, DDGS	$1\cdot10^{-4}$	-	$2.8\cdot10^{-4}$	-	-	-	$5.3\cdot10^{-5}$	-
Wood chips	$4.9\cdot10^{-4}$	$2.63\cdot10^{-4}$	$1.4\cdot10^{-3}$	$7.5\cdot10^{-4}$	-	-	$2.4\cdot10^{-4}$	$8\cdot10^{-6}$
MSW	$5.6\cdot10^{-4}$	-	$1.6\cdot10^{-3}$	-	-	-	$1.3\cdot10^{-4}$	-
Bioethanol	$1.24\cdot10^{-4}$	-	$3.5\cdot10^{-4}$	-	-	-	$2.7\cdot10^{-5}$	-
Boards, timber	$2.45\cdot10^{-4}$	$1.31\cdot10^{-4}$	$7\cdot10^{-4}$	$3.75\cdot10^{-3}$	-	-	$5.3\cdot10^{-5}$	$8\cdot10^{-6}$

*rail: 0.15 MJ/(m^3·km), road: 0.28 MJ/(m^3·km)

The environmental footprints for products are only assumed for digestate: CF 0.017 t/t and WPF 2.01 kg/t.

For each footprint $f \in FP$ out of six of them, a sequence of $(\mathrm{MINLP}-2)_{f,k}$ is performed where a relative footprint $(F^{r}_{f,k}(x))$ decreases from 1 to 0 by a suitable step-size, whilst the other footprints $ff \in FP \wedge ff \neq f$, are calculated. Thus a set of Pareto curves is obtained, one for each footprint. The main Pareto curves only are presented (see Figure 5-1) where a normalised footprint $(F^{r}_{f,k}(x))$ is obtained so that each footprint is divided by its maximal value obtained at MINLP-1 (Equation (5.9)). In Figure 5-1 profits vs. relative direct footprints are presented.

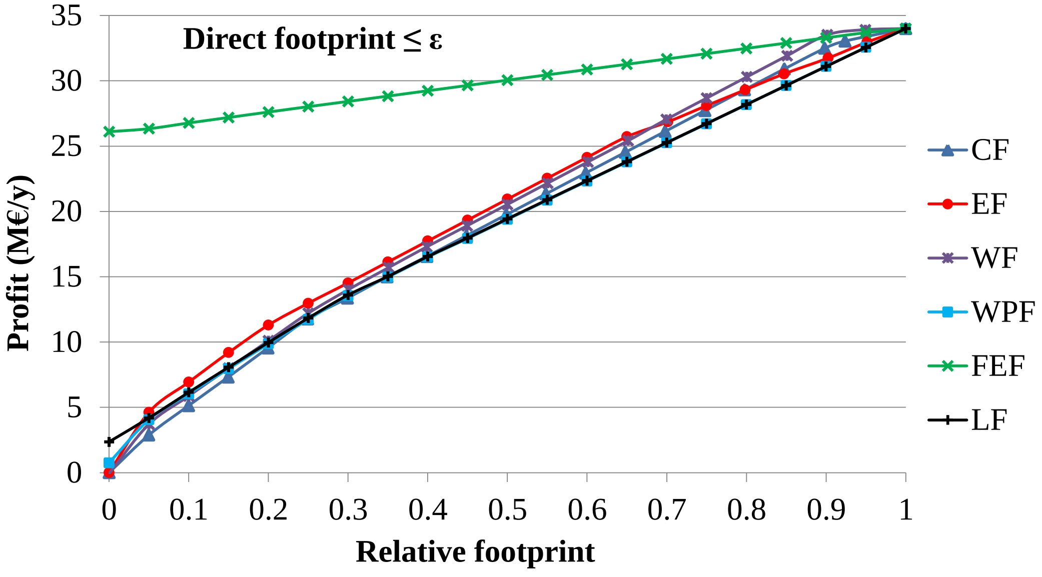


Figure 5-1. Profit vs. direct specific relative footprints (Čuček et al., 2012e)

It can be seen that especially the FEF differs from other footprints. The lower profit is obtained by lower FEFs, and that means that it is economically more preferable for producing energy rather than food. All the other footprints show similar behaviour with slight concave curvatures caused by the fact that by increasing the profit less and less sustainable alternatives could be selected. The profit increases at those lowest relative footprints steeper, by approximately 4.7 M€/y per 0.1 of relative footprint, whilst at the relative footprint 0.3 and higher only by approximately 2.9 M€/y per 0.1 of relative footprint.

Figure 5-2 presents profit vs. relative products flowrates when relative direct CF is simultaneously minimised by maximising the profit. The maximal flowrates of the products when their relative flowrates are 1, are: 243 GWh/y of electricity, 1.25 PJ/y of heat, 62.2 kt/y of ethanol, 3.65 kt/y of organic fertiliser, 48.1 kt/y of ethanol, 9.5 kt/y of boards, and 192 kt/y of corn.

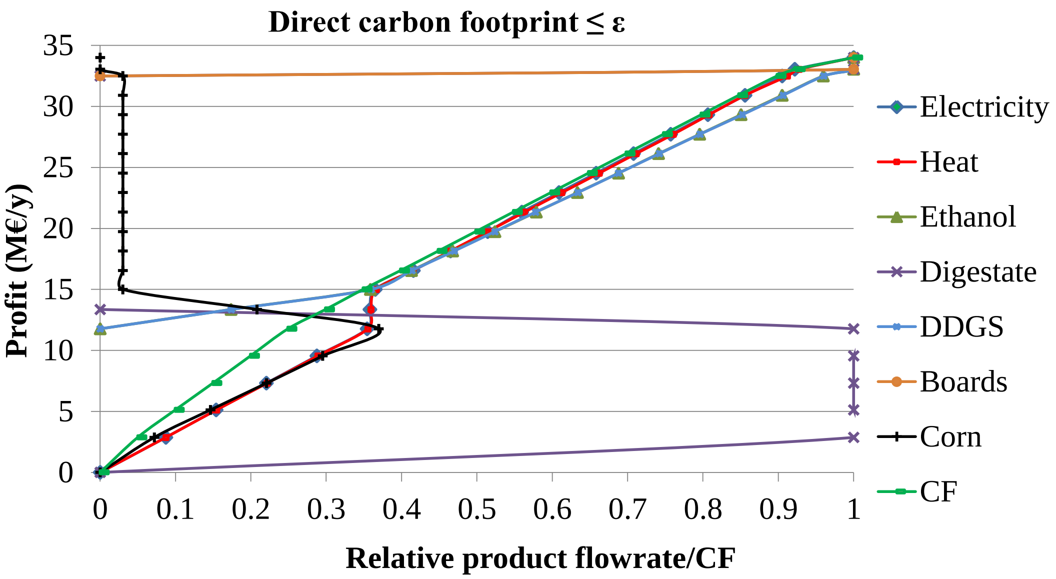


Figure 5-2. Profit vs. relative product flowrates when CF is minimised (Čuček et al., 2012e)

5.1.3.2 *Indirect and Total Footprints*

Total footprints are composed of direct and indirect footprints. Substitution factors should be defined in order to calculate the indirect footprints. The substitution factors for substituted vs. biomass products and their specific environmental footprints are presented in Table 5-4.

The calculated direct, indirect, and total footprints at MINLP-1 are presented in Table 5-5. These obtained values were set as maximal footprints, and when normalised, set to 1.

Table 5-4. Substitution factors and environmental footprints of substituted products

	Substitution factor	Water	Non-renewable energy consumption	Emissions to water	Emissions to air
Electricity mix/ electricity	1/1	1.26 t/MWh*	3.6 GJ/MWh	-	0.15 t/MWh
Heat mix/heat	1/1	0.175 t/GJ*	1 GJ/GJ	-	0.076 t/GJ
Gasoline/bioethanol	1/1.53	3 t/t	44.4 GJ/t	0.12 t/t	3.9 t/t
Corn/DDGS	1/1.2	900 t/t	15.9 GJ/t	0.032 t/t	0.154 t/t
Inorganic fertilizer/ digestate	1/34	150 t/t	40 GJ/t	1.15 t/t**	2.508 t/t
Steel/Boards	1/1	260 t/t	35 GJ/t	0.02 t/t	1.609 t/t

*the average WF of a mix of uranium, natural gas, coal and crude oil is 0.35 m^3/GJ

**the values for the amounts of used fertilisers are taken from (Frischknecht et al., 2007) for corn, production in the US

Table 5-5. Direct, indirect and total footprints obtained at MINLP-1

	Direct footprints	Indirect footprints	Total footprints
CF (t/(km^2·y))	118.66	-311.95	-194.3
WF (t/(km^2·y))	376,176.78	-39,210.75	337,290
EF (GJ/(km^2·y))	1,446.78	-4,906.72	-3,466.07
WPF (t/(km^2·y))	12.02	-6.47	5.55
LF (km^2/(km^2·y))	0.32	0	0.32
FEF (-)	0.38	0	0.38

It can be seen from Table 5-5 that by the replacement of biomass energy and bioproducts with conventional energy and products, CF and EF are reduced, whilst on the other hand the WF and WPF are increased. LF and FEF are zero for conventional fossil energy and therefore the total LF and FEF remains the same as for direct footprints.

When performing a sequence of $(\text{MINLP}-2)_{f,k}$ for relative total footprints, they decrease from 1 to 0 (for FEF, WF, WPF and LF – positive total footprints) or increase from -1 to 0 or even some positive value (for EF and CF – negative total footprints) until there is no feasible solution at zero profit, whilst again the other footprints $ff \in FP \wedge ff \neq f$, are calculated (see Figure 5-3). A set of Pareto curves is obtained, one for each footprint. Figure 5-3 presents the Pareto curves for profit vs. relative total footprints.

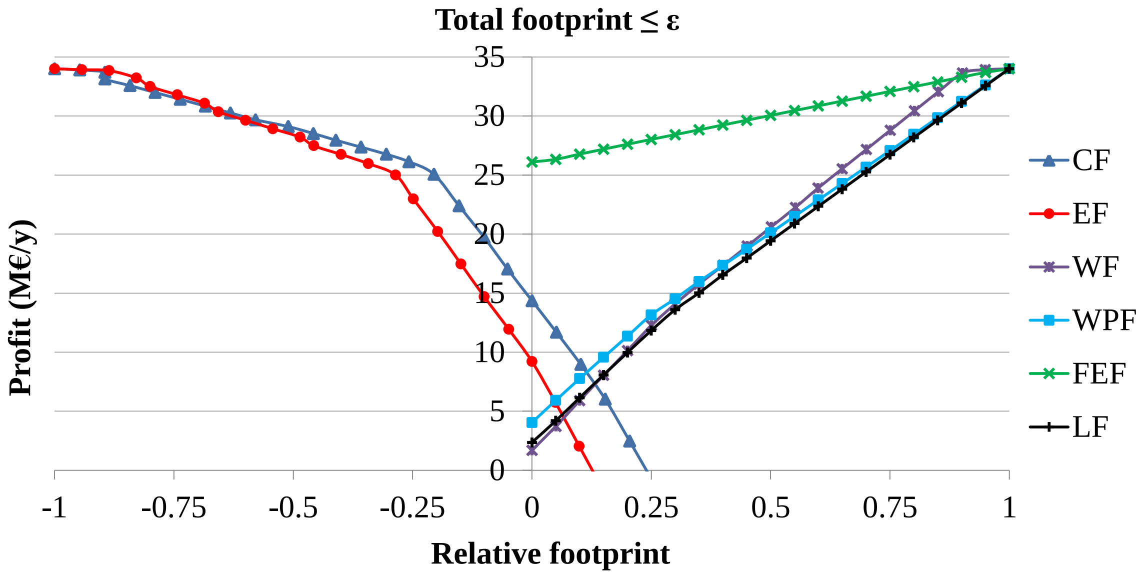


Figure 5-3. Profit vs. total specific relative footprints (Čuček et al., 2012e)

In the case of negative footprints, sets of non-trade-off optimal solutions are thus obtained, since relative footprints lower despite that profit increases.

It can be seen from Figure 5-3 that total CFs and EFs showed similar behaviour (mainly negative), from which it can be gathered that they are in relation. When using biomass energy instead of the currently mainly used fossil energy, the CFs and EFs are reduced. It should be noted that at zero total CF, a much higher profit (around 14.4. M€/y) is obtained compared to the direct alternative. Similar behaviour is also shown by WFs, WPFs and LFs, and are always positive, but their footprints, on the other hand, increased when using biomass energy. The reasons for this similar behaviour are that biomass energy requires more water, larger land areas, and some biomass also requires larger amounts of chemicals that cause pollution to water. All this is not the case for conventional energy (mainly fossil).

Figure 5-4 shows relative products flowrates vs. profit when total relative CF is simultaneously step-wise increased to zero profit with maximising the profit. The maximal flowrates of products are the same as for direct footprints. At zero CF, 145 GWh/y of electricity and 0.75 PJ/y of heat are generated (1.2 kWh/y of electricity and 6.03 MJ/y of heat as a direct alternative).

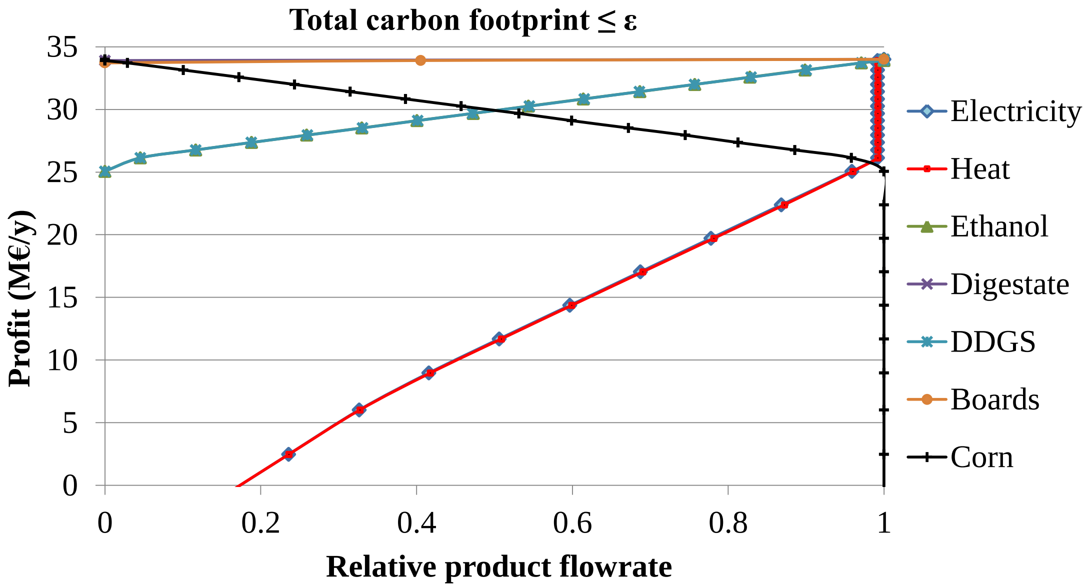


Figure 5-4. Profit vs. relative product flowrates where total CF is increased (Čuček et al., 2012e)

5.1.3.1 *Total Footprints Normalised by Direct Footprints*

When performing a sequence of $(\text{MINLP}-2)_{f,k}$ for relative total footprints, and when the obtained total footprints are divided by the values of the corresponding direct footprints obtained at MINLP-1 (see first column of Table 5-5) (total footprints normalised by direct ones instead of total ones, as shown in Figure 5-3), then some additional information could be gained about how much better or worse are the total footprints compared to the direct ones due to indirect environmental footprints.

Figure 5-5 shows Pareto curves for maximised profit vs. constrained relative total footprint by ε, and normalised by direct footprint. If a normalised footprint evaluated at a maximal value of profit has a value less than 1, this means that a total footprint has a lower value than its corresponding direct footprint and consequently, product's substitution helps to decrease the environmental burdening, especially when it achieves very negative values.

All the relative normalised footprints, except LF and FEF, are improved compared to their direct footprints. LF and FEF are the same as their direct footprints, as they have no indirect footprints. Biomass production also requires larger land areas (contributes to LF) and production of energy from food-intended crops consumes larger amounts of these crops (contributes to FEF), which is not the case when using conventional fossil-based energy. EF and CF especially are very negative, and therefore substantially unburden the environment when biomass energy is used instead of the currently used energy. Positive, but less than 1, are the relative normalised footprints for WPF and WF, meaning that their burdens decrease compared to their direct impacts, but do not diminish.

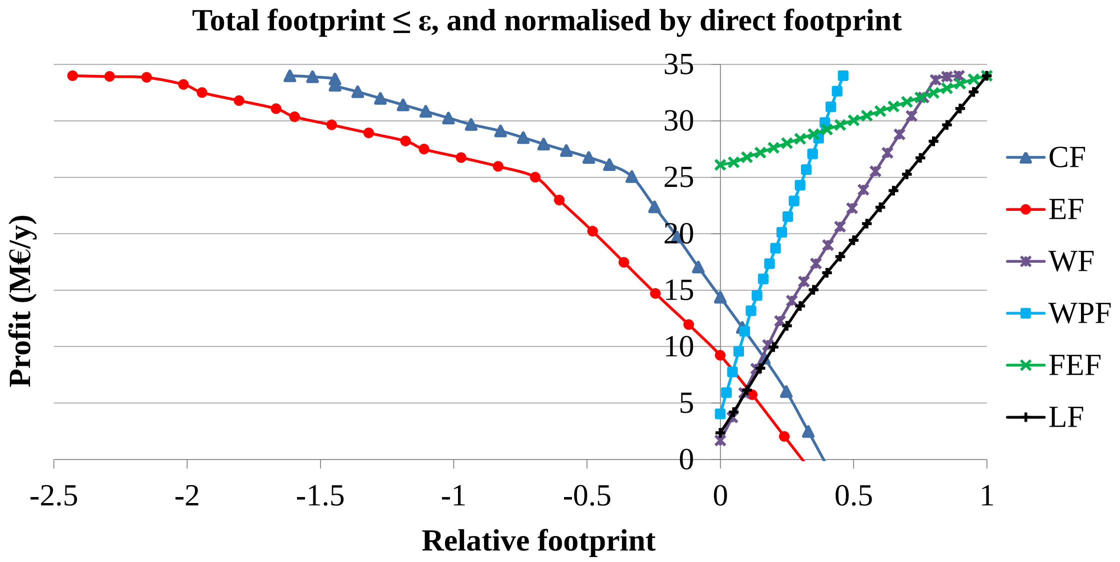


Figure 5-5. Profit vs. total specific footprints normalised by direct footprints

The absolute values for total footprints regarding maximal profit at the ends of their Pareto curves (see Figure 5-5), are those values presented in the last column in Table 5-5. These total footprint curves can be directly compared to the direct footprint ones in Figure 5-1, as all of them are normalised using the same footprint values.

5.2 Direct, Indirect, and Total Sustainability Indexes

The aim of this part of the work is defining a method for identifying sustainable solutions, where economic, and/or environmental, and/or social aspects would be simultaneously included within the objective function. Different sustainability indicators are compiled within a single index (relative sustainability index, RSI) using certain weights. In addition to the direct (burdening), indirect (unburdening) effects are also considered from the life-cycle perspective.

The relative direct sustainability index (RDSI) is only composed of direct impacts on the environment and society. RDSI is always positive (negative for the environment). RDSI usually ranges from 1, for its worst possible value, to 0 as its best possible value. Relative indirect sustainability index (RISI) considers the indirect effects, those sets of impacts that indirectly unburden or benefit the environment when e.g. waste is utilised instead of being deposited, or environmentally-benign raw materials, products or services are used instead of harmful ones (the substitution, and therefore it refers to current situations). Relative total sustainability index (RTSI) besides burdening also includes unburdening. RTSI ranges from -1 or even from more negative values (positive for the environment), to 0. Values of RSI < 0 are beneficial, while RSI > 0 are bad for the environment, and the higher the value, the worse for the environment.

A systematic approach was applied in order to define direct, indirect, and total effects. For this purpose, different sets were defined for raw materials and products $(p \in R_{\mathrm{B}} \cup R_{\mathrm{UNB}} \cup P_{\mathrm{B}} \cup P_{\mathrm{UNB}})$.

Sets for raw materials:

i) R_{B} – set of those raw materials that only burden the environment if processed, e.g. fossil fuels, since they were stored under the Earth's crust over millions of years and now moved into the biosphere; crops, since they use chemicals and fuels in relation to their production; water, since if processed it should be cleansed, residues, since they control the erosion, and/or are organic fertilisers, etc.

ii) R_{UNB} – set of those raw materials that also unburden or benefit the environment when used; e.g. the utilisation of waste (industrial wastewater – IW, manure, sludge, etc.), since their direct harmful impact on the environment is thus avoided; but some burdens are still released, e.g. when transporting to the plant.

Sets for products:

i) P_{B} – set of those products that only burden the environment in relation to processing, disposal, and transportation.

ii) P_{UNB} – set of those products that also unburden or benefit the environment, e.g. if they are substitutes for harmful products; but note that some burdens are still released, mainly due to processing and transportation.

5.2.1 Direct, Indirect, and Total Sustainability Indicators

5.2.1.1 Direct Sustainability Indicator

The direct sustainability indicator $(I_o^{\mathrm{d}},\ o \in O)$ represents the burdening of the environment. It is defined as the sum of different burdens, where each burden is further defined as a product between the raw materials' or products' (p) mass, molar, volume, energy, etc. flowrate $(q_p^m\,/\,(\mathrm{t/y,\ GJ/y,\ ...}))$, and its specific indicator $(I_{o,p}^{\mathrm{s}}\,/\,(\mathrm{kg/t,\ ha/t,\ ...}))$:

$$I_o^{\mathrm{d}} = \sum_{p \in R_{\mathrm{B}} \cup R_{\mathrm{UNB}} \cup P_{\mathrm{B}} \cup P_{\mathrm{UNB}}} q_p^m \cdot I_{o,p}^{\mathrm{s}} + \sum_{p \in R_{\mathrm{B}} \cup R_{\mathrm{UNB}} \cup P_{\mathrm{B}} \cup P_{\mathrm{UNB}}} q_p^m \cdot l_p \cdot D_p \cdot I_{o,p}^{\mathrm{s,tr}} \qquad \forall o \in O \qquad (5.10)$$

This summation is performed over all raw materials and products, as all of them contribute to the burdening. The second term represents burdening due to transportation, where the p^{th} flowrate is multiplied by an inverse of the load factor, l_p, the distance, $(D_p\,/\,\mathrm{km})$, and a specific sustainability indicator for transportation, $I_{o,p}^{\mathrm{s,tr}}$ /(kg/(t·km), kg/(m^3·km), …). Note that the inverse of the load factor is set to 2 when the transport is loaded in one direction and empty in the other. The summation is accomplished for each $o \in O$, a sustainability (economic and/or environmental and/or social) indicator or objective.

I_o^{d} includes those burdens that originate from the extraction of raw materials, the disposal of harmful products, or from the purification of polluted products, and from all transportation and distribution paths within the supply chain.

5.2.1.2 Indirect Sustainability Indicator

The indirect sustainability indicator (I_o^{ind}, $o \in O$) is defined as the sum of all the positive impacts of unburdening the environment:

$$I_o^{\text{ind}} = -\sum_{p\in R_{\text{UNB}}} q_p^m \cdot I_{o,p}^{\text{s}} - \sum_{p\in P_{\text{UNB}}} q_p^m \cdot f_p^{S/P_{\text{UNB}}} \cdot I_{o,p}^{\text{s}} \qquad \forall o \in O \tag{5.11}$$

The first term represents unburdening of the environment due to the use of environmentally-harmful raw materials that are now processed rather than being deposited. Note that this unburdening is equivalent to the negative burden if deposited. The second term represents the unburdening when a product substitutes a conventional harmful product, e.g. bioethanol vs. gasoline. Symbol $f_p^{S/P_{\text{UNB}}}$ (/) denotes the substitution factor, defined as the ratio between the quantity of conventional product S, and the quantity of produced biomass product P_{UNB}.

5.2.1.3 Total Sustainability Indicator

The total sustainability indicator (I_o^{t}, $o \in O$) is defined as the sum of the burdening and unburdening of the environment (and society):

$$I_o^{\text{t}} = I_o^{\text{d}} + I_o^{\text{ind}} \qquad \forall o \in O \tag{5.12}$$

I_o^{t} becomes negative when the unburdening surpasses the burdening. The more negative the total indicator, the more sustainable the system, and vice versa.

5.2.2 Relative Sustainability Index

As sustainability includes environmental, economic, and social dimensions (Jørgensen et al., 2008), the RSI is composed of economic, environmental, and social indicators (Tallis et al., 2002). As these indicators have different units, they cannot be composed unless they are normalised. They can be normalised either on the basis of a well-known reference system, on the basis of the best available techniques – BAT (Kravanja et al., 2005), or on the basis of the referenced solution, obtained by SOO of the economic profit (superscript 0). The SOO step corresponds to the first MI(N)LP step, and MOO to the second MI(N)LP step of the of LCA-based synthesis. The aim of the first step is to provide a reference solution for the normalisation of the indicators.

5.2.2.1 Economic Indicators

A key element of sustainability is usually the economic performance of a product, service or activity. As economic indicators, either yearly profit (P) or the net present value (NPV, W_{NP}) can be used, and are maximised. Another possible relevant indicator is also the operating cost, which is minimised. If e.g. P or W_{NP} of a studied alternative is compared to a given base-case, P^0 or W_{NP}^0, relative profit (RP) and relative NPV (RW_{NP}) are obtained:

$$RP = \frac{P}{P^0}; \qquad RW_{\mathrm{NP}} = \frac{W_{\mathrm{NP}}}{W_{\mathrm{NP}}^0} \tag{5.13}$$

5.2.2.2 Environmental Indicators

Environmental metrics should provide a balanced view of inputs' (resource usage) and outputs' (products, services, and activities produced, and the emissions, effluents and waste) environmental impacts. Environmental indicators are typically grouped into resource usage indicators (material, energy, water, and land) and pollution indicators (global warming, atmospheric acidification, photochemical smog formation, human health effect, etc.) (Tallis et al., 2002). Often, the optimal solution at the first MI(N)LP step (base-case solution) produces those environmental indicators that are reference points for the second step, which then yields a sustainable solution.

5.2.2.3 Social Indicators

The social indicators (SIs) deal with measuring the quality of life. SIs relate to housing and ecology, employment, human rights, poverty, education, health and safety etc., and are usually overlooked since their assessment is not a straightforward task (Kravanja et al., 2005).

5.2.3 Implementation of the Relative Sustainability Index

When the indicators (I_o) of a studied alternative and are compared to those of the selected base-case (I_o^0), relative indicators are obtained, which can then be compiled into a RSI, by suitable weighting factors $(w_o, \ \sum_{o \in O} w_o = 1)$:

$$\mathrm{RSI} = \sum_{o \in O} w_o \cdot \frac{I_o}{I_o^0} \tag{5.14}$$

If only the direct effects on the environment and society are considered, then the RDSI is obtained – Equation (5.15). In addition, if indirect effects are considered, the RTSI is obtained – Equation (5.16) that shows how much better (or even worse) is RTSI than RDSI:

$$\mathrm{RDSI} = \sum_{o\in O} w_o \cdot \frac{I_o^{\mathrm{d}}}{I_o^{\mathrm{d},0}} \tag{5.15}$$

$$\mathrm{RTSI} = \sum_{o\in O} w_o \cdot \frac{I_o^{\mathrm{d}} + I_o^{\mathrm{ind}}}{I_o^{\mathrm{d},0}} = \sum_{o\in O} w_o \cdot \frac{I_o^{\mathrm{t}}}{I_o^{\mathrm{d},0}} \tag{5.16}$$

The higher the quotient between the total and direct effects (this is the case of alternatives that significantly unburden the environment); the more this indicator changes the RTSI, and lowers the value of RTSI.

5.2.3.1 Two-Step LCA-based MINLP Synthesis

A two-step MINLP system synthesis is performed where an economically-effective synthesis is carried out during the first step in order to obtain a solution, which is then considered as a base-case or referenced solution for the multi-objective MINLP synthesis, as performed during the second step.

When the ε-constraint method is applied, a set of non-inferior Pareto optimal solutions are thus generated. The aim is to obtain solutions that are economically more efficient and yet environmentally less harmful than the base-case solution. However, with this approach, the LCA practitioner cannot avoid subjective weighting between different environmental and/or social indicators.

The synthesis problem, where e.g. a sequence of N problems (MINLP-RSI)$_k$ is performed as a maximisation of profit (P) subjected to a single RSI, takes the following form:

$$\begin{aligned}
&\max_{x,y} P_k = c^{\mathrm{T}} y + f(x) \\
&\text{s.t.} \quad Ay + h(x,y) = 0 \\
&\qquad By + g(x,y) \le 0 \\
&\qquad \mathrm{RSI}(x) \ge \varepsilon_k \;\; (\mathrm{RSI}(x) \le \varepsilon_k) \\
&\qquad (x^{\mathrm{LO}} \le x \le x^{\mathrm{UP}}) \in X \subset R^n,\; y \in Y = \{0,1\}^m \\
&\qquad \varepsilon_k = \varepsilon_{k-1} + \Delta\varepsilon \;\; (\varepsilon_k = \varepsilon_{k-1} - \Delta\varepsilon),\; \Delta\varepsilon = \frac{1}{N},\; \varepsilon_1 = 1,\; k \in K = \{1,\dots,N+1\}
\end{aligned} \tag{MINLP-RSI$_k$}$$

RSI increases (decreases) sequentially by a suitable step-size until there is no feasible solution. Pareto non-inferior solutions are obtained with RSI > 0 and non-trade-off optimal solutions with RSI < 0. In those cases when profit does not decrease or increase monotonically with RSI, ε-equality constraint can be used rather than the inequality constraint.

5.2.4 Illustrative Example

The presented approach is illustrated through a case study that is comprised of integrated bioprocesses for the production of biogas from organic and animal wastes, including the option of a rendering plant (Drobež et al., 2011). The superstructure of the heat-integrated biogas production supply chain is shown in Figure 5-6.

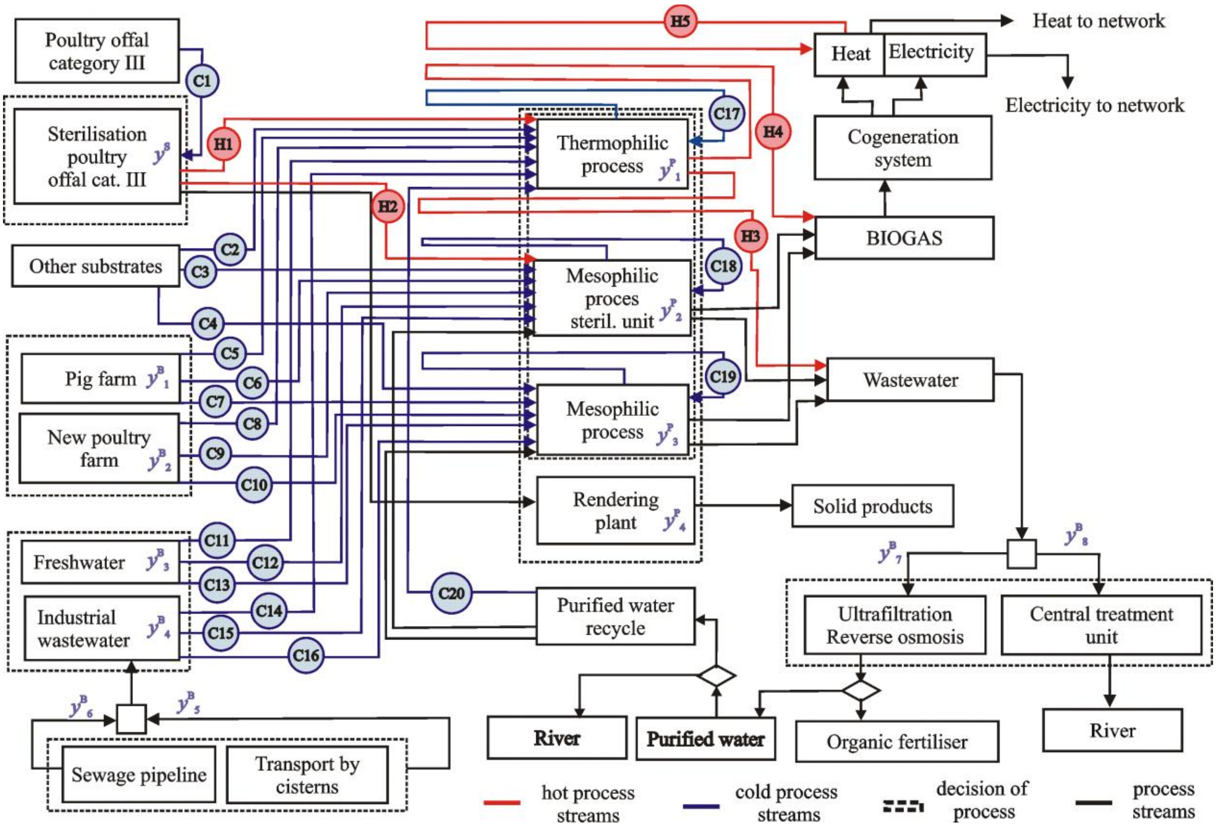


Figure 5-6. Superstructure of heat integrated biogas production supply chain (modified from (Drobež et al., 2011))

In this dissertation, only a short description of the superstructure and synthesis of biogas production supply chain will be provided, since this synthesis was mostly performed by Rozalija Drobež. She presented a detailed description of the synthesis model and superstructure in (Drobež et al., 2009), including simultaneous heat integration (Drobež et al., 2011), and piecewise linear approximation of non-linear terms (Drobež et al., 2010). Now it has been upgraded by the above-described MOO approach based on sustainability metrics using RDSI and replaced RTSI.

This superstructure of a biogas production supply chain (see Figure 5-6) involves various biogas production options and different auxiliary facilities. The animal manure, corn silage, grape skins, offal, and organic wastes from a meat company are utilised by AD under mesophilic or thermophilic conditions, and the animal offal could be alternatively processed by a rendering plant. The other auxiliary facilities involve various options for the selection of inlet materials, which could be transported from the existing or potential farms, e.g. either the existing pig farm could be reconstructed or adapted into a new poultry farm. Also different options for water supplies, for the transportation of IW, and various options for wastewater treatments are included, e.g. an additional water source could either be freshwater from a local well or IW from other meat-processing industries, the IW could either be transported by the pipelines or by cisterns, and the wastewater could either be purified within a central treatment unit within an open water system, or by the use of ultrafiltration and reverse osmosis within a closed water system. The produced biogas could be converted into heat and electricity within combined heat and power (CHP) plants. The solid products from the rendering plant – meat, bone and poultry by-product meal could be sold as pet food, and the tallow used as a material for the production of soaps, biodiesel, etc. The wastewater from the biogas plant could either be purified and recycled or discharged into the environment, whilst the by-product could be sold as organic fertiliser.

This superstructure model considers a simplified simultaneous synthesis and HI (Duran and Grossmann, 1986), which uses the pinch location method. The circles within the superstructure in Figure 5-6 represent 5 hot (H1-H5) and 20 cold (C1-C20) process streams. Hot streams H1-H5 include sterilised inlet streams towards the AD process, and outlet streams from the thermophilic process and cogeneration unit. Cold streams C1-C20 involve waste material entering the sterilisation unit, substrates from different farms, supplied water (freshwater, IW and/or recycled water), and the heat stream required for AD.

The model described with Equations (5.10) – (5.16) is used in order to calculate RDSI and RTSI. A comprehensive analysis is carried out that includes all stages of the biogas production. As the ε-constraint method is applied with economic indicator (profit) in the objective function, the RSI is composed of environmental indicators only. For this illustrative example, the SIs are undefined, since their assessment would not be a straightforward task.

A new set O for environmental indicators is defined using elements $o \in O = \left\{ \text{CF, LF, WS, NF} \right\}$. The CF includes the exclusive direct and indirect CO_2 emissions, as proposed by (Wiedmann and Minx, 2008). The LF represents the land area used to grow biomass (Kissinger and Gottlieb, 2010). The WS stands for the mass flow-rate of water stream. The NF is a measurement of the amount of reactive nitrogen (N_r, all N species except N_2) released into the environment (N-Print, 2011). N_r includes the different, more abundant, nitrogen species, NO_x (NO and NO_2, expressed as NO_2), N_2O, NO_3^-, and NH_3.

5.2.4.1 Input Data

The input data for calculating the sustainability index, are presented in Table 5-6 – Table 5-10. It should be noted that the burdens associated with constructing a biogas and rendering plant, and the manufacturing of machinery, were assumed to be negligible because they are used over a plant's entire life-time. The burdens associated with human labour are not considered for reasons of simplification. From the process only the burdens associated with the purchased electricity are assumed.

Table 5-6 shows those specific environmental burdens (burden per unit) associated with raw materials and purchased electricity $(I_{o,p}^{s})$. Those specific environmental unburdens (unburden per unit) associated with raw materials are unconsidered to be on the conservative side.

Table 5-6. Environmental impacts associated with raw materials

Raw material	Indicator *o*			
	CF (kg CO_2/t)	LF (ha/t)	WS (kg H_2O/t)	NF (kg N/t)
Direct sustainability indicator for R_B				
Maize silage	16.967	0.023	817.51	1.220
Water	0	0	1,000	0
Purchased electricity*	113.82	0	4,987.4	$8.35 \cdot 10^{-2}$
Direct sustainability indicator for R_{UNB}				
IW from poultry farm	0	0	990	0
IW from the prepared meals factory	0	0	998	0
IW from meat-processing industry	0	0	999	0
Pig manure	0.052	0	953	$3.28 \cdot 10^{-5}$
Poultry manure – new farm	0.052	0	503	$3.28 \cdot 10^{-5}$
Cattle manure	0.052	0	923	$3.28 \cdot 10^{-5}$
Poultry manure – broilers	0.052	0	503	$3.28 \cdot 10^{-5}$
Poultry manure – layer	0.052	0	403	$3.28 \cdot 10^{-5}$
Poultry manure – breeding	0.052	0	203	$3.28 \cdot 10^{-5}$
Liquid pig manure	0.052	0	983	$3.28 \cdot 10^{-5}$
Animal offal at location 2	0	0	820	0
Animal offal at location 4	0	0	820	0
Bones at location 2	0	0	820	0
Bones at location 4	0	0	820	0
Slaughterhouse waste at location 2	0	0	820	0
Slaughterhouse waste at location 4	0	0	820	0
Blood	0	0	993	0
Waste from the production of poultry meat	0	0	820	0
Poultry litter	44.301	0.228	514.14	0.231
Hatchery waste	0	0	700	0
Grape skins	0	0	600	0
Flotate at location 2	0	0	900	0
Flotate at location 4	0	0	900	0

*instead of per ton, indicators are defined per GJ

Table 5-7 shows the locations of raw materials and products, the distances from the locations of the raw materials to the location of the biogas and rendering plant, and the distances of the products from the end-usage (D_p).

Table 5-7. Locations of raw materials, products, and distances

Raw material	Location	Distance (km)
Distance of R_B to plant		
Maize silage	Surroundings of location 1	5
Water	Near the plant	0
Distance of R_{UNB} to plant		
IW from poultry farm	Location 1	2
IW from the prepared meals factory	Location 2	7
IW from meat-processing industry	Location 2	10
Pig manure	Location 1	1
Poultry manure – new farm	Location 1	1
Cattle manure	Location 3	20
Poultry manure – broilers	Location 1	1
Poultry manure – layer	Location 1	1
Poultry manure – breeding	Location 1	1
Liquid pig manure	Location 1	1
Animal offal at location 2	Location 2	10
Animal offal at location 4	Location 4	140
Bones at location 2	Location 2	10
Bones at location 4	Location 4	140
Slaughterhouse waste at location 2	Location 2	10
Slaughterhouse waste at location 4	Location 4	140
Blood	Location 2	10
Waste from the production of poultry meat	Location 2	10
Poultry litter	Location 1	2
Hatchery waste	Location 1	2
Grape skins	Surroundings of location 2	20
Flotate at location 2	Location 2	10
Flotate at location 4	Location 4	140
Distance of P_B to end-usage		
Wastewater	Biogas plant	10
Distance of P_{UNB} to end-usage		
Organic fertiliser	Biogas plant	10
Meat and bone meal	Rendering plant	200
Tallow	Rendering plant	200
Poultry by-product meal	Rendering plant	200

The raw materials are at different distances from the plants and different means of transport have to be used. However, for reasons of simplification, all specific environmental indicators $(I^{\mathrm{s,tr}}_{o,p})$ are assumed to be the same per t·km, CF – 0.257 kg CO_2/(t·km), LF – 0 ha/(t·km), WS – 1.744 kg H_2O/(t·km), and NF – $2.9 \cdot 10^{-4}$ kg N/(t·km).

The specific burdens for the produced products from biogas and the rendering plants $(I^{\mathrm{s}}_{o,p})$ are all zero or neglected, except NF for organic fertiliser, which is 0.052 kg N/t.

Table 5-8 presents the substitution factors relating to the replacement of conventional, mainly non-renewable products, with renewable products. The substitution factor is defined as the ratio between the quantity of conventional product, and the quantity of biogas and rendering plants' product.

Table 5-8. Substituted products with biomass products and their ratios

Product (P_{UNB})	Substituted product (S)	Substitution factor ($f_p^{S/P_{\mathrm{UNB}}}$)
Heat	Heat from natural gas	1/1
Electricity	Electricity mix	1/1
Organic fertiliser	Inorganic fertiliser	1/34
Meat and bone meal	Protein concentrates	1/1
Tallow	Palm oil	1/1
Poultry by-product meal	Protein concentrates	1/1

Table 5-9 shows the indirect (unburdening) specific environmental effects, caused due to the replacement of conventional harmful products $(I_{o,p}^{\mathrm{s}})$.

Table 5-9. Indirect environmental indicators associated with substituted products

	Indicator *o*			
Substituted product (S)	CF (kg CO_2/t)	LF (ha/t)	WS (kg H_2O/t)	NF (kg N/t)
Heat from natural gas	67.32	0	76.63	0.0137
Electricity mix	113.82	0	4,987.40	0.0835
Inorganic fertiliser	2,424.10	0	121,420.00	3.1202
Palm oil	864.17	0	228,010.00	5.9415
Protein concentrates	117.13	0	966.39	0.3221

Each part of Equations (5.10) – (5.12) is comprised either of raw materials or products flowrates, both being optimisation variables in the ε-constraint method. Their values from the economically-optimal solution are presented in Table 5-10. The flowrate of purchased electricity is 21,598.42 GJ/y.

5.2.4.1 Economically-Optimal Solution – MINLP-1

At MINLP-1 the economic profit is maximised and the reference values for I_o^{d}, I_o^{ind}, and I_o^{t} are calculated, which are then used at MINLP-2 to normalise the RDSI and RTSI.

The optimal solution consists of an economic profit of 3.668 M€/y. In terms of biogas production (see Figure 5-7) it includes the use of a thermophilic process that would convert the liquid pig manure and other substrates, using no additional processed water. A reconstruction of the existing pig farm and a closed water system with ultrafiltration and reverse osmosis are selected. In the optimal solution the rendering process is deselected.

Table 5-10. Variables set for the economically-optimal biogas production

Raw material	Flow-rate q_p^m (t/y)	Product	Flow-rate, q_p^m (t or GJ/y)
Flow-rate of R_{B}		*Flow-rate of* P_{B}	
Maize silage	8,000.00	Wastewater	-
Water	-		
Flow-rate of R_{UNB}		*Flow-rate of* P_{UNB}	
IW from poultry farm	-	Heat	155,235.49
IW from the prepared meals factory	-	Electricity	131,087.77
IW from meat-processing industry	-	Organic fertiliser	27,658.54
Pig manure	5,000.00	Meat and bone meal	-
Poultry manure – new farm	-	Tallow	-
Cattle manure	18,000.00	Poultry by-product meal	-
Poultry manure – broilers	923.50		
Poultry manure – layer	2,375.00		
Poultry manure – breeding	789.50		
Liquid pig manure	60,001.20		
Animal offal at location 2	12,822.00		
Animal offal at location 4	1,240.00		
Bones at location 2	1,300.00		
Bones at location 4	80.00		
Slaughterhouse waste at location 2	3,900.00		
Slaughterhouse waste at location 4	600.00		
Blood	2,460.00		
Waste	520.00		
Poultry litter	3,126.48		
Hatchery waste	400.00		
Grape skins	625.00		
Flotate at location 2	510.00		
Flotate at location 4	190.00		

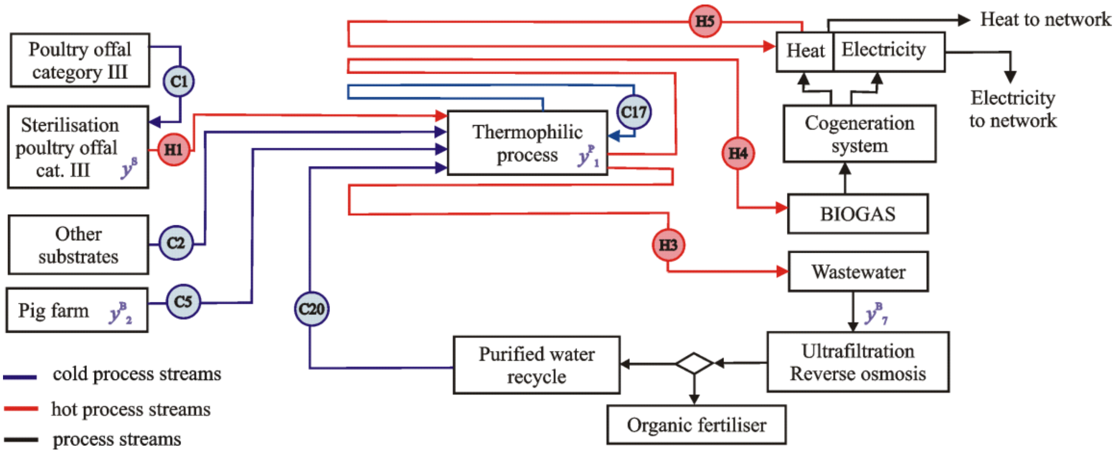


Figure 5-7. Optimal process obtained by the maximisation of economic profit (modified from (Čuček et al., 2012a))

By applying data from Table 5-6 – Table 5-10 it is possible to calculate I_o^{d}, I_o^{ind} and I_o^{t} of the economically-optimal solutions. The results obtained for each part of Equations (5.10) and (5.11) are presented in Table 5-11 for direct and indirect sustainability indicators.

Table 5-11. Calculated environmental impacts

	Indicator *o*			
	CF (kt CO_2/y)	LF (kha/y)	WS (kt H_2O/y)	NF (t N/y)
Direct sustainability indicator (I_o^{d})				
$\sum_{p\in R_{\mathrm{B}}} q_p^m \cdot I_{o,p}^{\mathrm{s}}$	2.594	0.183	114.260	11.565
$\sum_{p\in R_{\mathrm{UNB}}} q_p^m \cdot I_{o,p}^{\mathrm{s}}$	0.143	0.714	104.098	0.724
$\sum_{p\in P_{\mathrm{B}}} q_p^m \cdot I_{o,p}^{\mathrm{s}}$	0	0	0	0
$\sum_{p\in P_{\mathrm{UNB}}} q_p^m \cdot I_{o,p}^{\mathrm{s}}$	0	0	0	1.442
$\sum_{p\in R_{\mathrm{B}}} q_p^m \cdot 2 \cdot D_p \cdot I_{o,p}^{\mathrm{s,tr}}$	0.021	0	0.140	0.023
$\sum_{p\in R_{\mathrm{UNB}}} q_p^m \cdot 2 \cdot D_p \cdot I_{o,p}^{\mathrm{s,tr}}$	0.493	0	3.346	0.556
$\sum_{p\in P_{\mathrm{B}}} q_p^m \cdot 2 \cdot D_p \cdot I_{o,p}^{\mathrm{s,tr}}$	0	0	0	0
$\sum_{p\in P_{\mathrm{UNB}}} q_p^m \cdot 2 \cdot D_p \cdot I_{o,p}^{\mathrm{s,tr}}$	0.142	0	0.965	0.160
SUM	3.393	0.897	222.809	14.471
Indirect sustainability indicator (I_o^{ind})				
$\sum_{p\in R_{\mathrm{UNB}}} q_p^m \cdot I_{o,p}^{\mathrm{s}}$	0	0	0	0
$\sum_{p\in P_{\mathrm{UNB}}} q_p^m \cdot f_p^{S/P_{\mathrm{UNB}}} \cdot I_{o,p}^{\mathrm{s}}$	-27.343	0	-764.456	-15.599
SUM	-27.343	0	-764.456	-15.599
Total sustainability indicator (I_o^{t})	-23.950	0.897	-541.647	-1.129

The obtained values of I_o^{d}, I_o^{ind} and I_o^{t} at the MINLP-1 are summarised in Table 5-12.

Table 5-12. Direct, indirect and total sustainability indicators at MINLP-1

	Direct indicator (I_o^{d})	Indirect indicator (I_o^{ind})	Total indicator (I_o^{t})
CF (kt CO_2/y)	3.393	-27.343	-23.950
LF (kha/y)	0.897	0	0.897
WS (kt H_2O/y)	222.809	-764.456	-541.647
NF (t N/y)	14.471	-15.599	-1.129

It can be seen from Table 5-12 that the indirect sustainability indicators, except LF, are prevalent and therefore the total sustainability indicators are negative (positive for the environment). This means that from the environmental point of view (from CF, WS, and NF) it is better to produce products from AD (heat, electricity, and organic fertiliser) instead of the conventional currently-used products (electricity mix, heat from natural gas, and inorganic fertiliser) and thus allow for conservation of the environment.

In terms of CF, the main negative contributor is the power consumption of the plant itself, as the electricity is purchased from the grid. Consequently, the replaced power and heat contribute the most to unburdening the environment. In terms of LF, the only contributors are corn silage and corn stover, where corn stover has the higher LF. The replaced products do not have LF, therefore indirect LF is zero. In terms of direct WS, the major water users are raw materials for biogas production (especially liquid pig manure), and electricity purchased from the grid (Slovenian specific electricity supply mix). The major unburdening effect is the replacement of the electricity supply mix with the same amount of electricity from biogas. In terms of direct NF, the corn silage is the main contributor, and the purchased electricity the second contributor. Again, the replaced power contributes most to unburdening the environment.

5.2.4.2 Multi-Objective Synthesis at MINLP-2

During the second MINLP step (MINLP-2), a sequence of (MINLP-RSI)$_k$ problems is carried-out and multi-objective synthesis performed using the ε-constraint method, where economic performance is the main objective, and as an additional objective, RSI is constrained by ε. RDSI decreases from a maximum $(\varepsilon = 1)$ to a minimum value $(\varepsilon = 0$, or until an infeasible solution). Since RTSI is defined as a weighted-sum of the total sustainability indicators, divided by the corresponding direct sustainability indicators, the RTSI usually decreases from the minimum value at MINLP-1 to a maximum value obtained by the zero profit or by infeasible solution. Pareto optimal solutions are obtained between the economic and environmental objectives.

The intention is to obtain solutions with considerably smaller CF; therefore it is decided to take the weighting factor for the CF 1/2, and also for all the other environmental indicators together (LF, WS and NF) 1/2:

$$\mathrm{RSI} = \frac{1}{2} \cdot \frac{\mathrm{CF}}{\mathrm{CF}^0} + \frac{1}{2} \cdot \frac{1}{3} \cdot \left(\frac{\mathrm{LF}}{\mathrm{LF}^0} + \frac{\mathrm{WS}}{\mathrm{WS}^0} + \frac{\mathrm{NF}}{\mathrm{NF}^0} \right) \tag{5.17}$$

All the indicators are normalised by their values as obtained during the first step (superscript 0). The referenced values are direct sustainability indicators $(I_o^{\mathrm{d},0})$, and are: CF^0 = 3.393 kt CO$_2$/y, LF^0 = 0.897 kha/y, WS^0 = 222.809 kt H$_2$O/y, and NF^0 = 14.471 t N/y (see Table 5-12).

Equation (5.17) is used in order to calculate RDSI and RTSI. At an economically-optimal solution, the RDSI is equal to 1, since CF = CF^0, ALF = ALF^0, WS = WS^0, and NF = NF^0:

$$\text{RDSI} = \frac{1}{2}\cdot\frac{3.393}{3.393} + \frac{1}{2}\cdot\frac{1}{3}\cdot(\frac{0.897}{0.897} + \frac{222.809}{222.809} + \frac{14.471}{14.471}) = 1.00$$

RTSI is defined as weighted total effects divided by direct effects:

$$\text{RTSI} = \frac{1}{2}\cdot\frac{(-23.950)}{3.393} + \frac{1}{2}\cdot\frac{1}{3}\cdot(\frac{0.897}{0.897} + \frac{(-541.647)}{222.809} + \frac{(-1.129)}{14.471}) = -3.74$$

Note that for this specific case RDSI = 1.00 corresponds to the extreme points of the Pareto curve for RDSI, and RTSI = -3.74 to the extreme point of the non-trade-off solution curve for RTSI, see Figure 5-8.

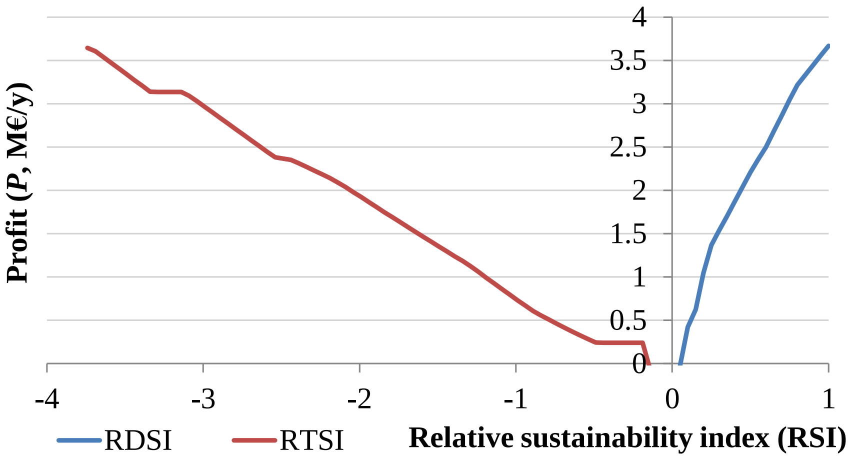


Figure 5-8. A Pareto curve for RDSI and a set of non-trade-off solutions for RTSI (Kravanja and Čuček, 2013)

The Pareto optimal solutions are obtained for RDSI (Figure 5-8) from the maximum economic profit (3.668 M€/y) and maximal RDSI (RDSI = 1), to a solution with the RDSI by the zero profit (RDSI ≈ 0.05). The most economically-optimal solution is the environmentally the worst one, and vice versa. By ‘improving’ the RDSI, the profit become lower and lower, and the best solution from the environmental perspective is the one where the profit is 0 and nothing is produced.

By only considering the direct effects, the obtained solutions are wrong as they indicate that biogas production is unsustainable. By also taking into account the indirect effects in RTSI, the ‘opposite’ solutions are obtained, namely biogas production is a sustainable alternative along the whole set of non-trade-off solutions, within the whole range of profits – from the maximum economic profit (3.668 M€/y) and minimal RTSI (RTSI ≈ -3.74), to a solution with the RTSI having a zero profit (RTSI ≈ -0.15). These solutions are non-trade-off solutions, since with increasing profit, even more and more sustainable solutions are obtained.

The economically-optimal solution is the environmentally-optimal solution from the RTSI, and comprises the selection of the thermophilic process and the closed water system (see Figure 5-7). From RDSI ≈ 0.05, the mesophilic process and, again the closed water system are selected, and from RTSI ≈ -0.15 the thermophilic process and the open water system are selected.

Figure 5-9 shows how the product flowrates change with the decreasing of the RDSI.

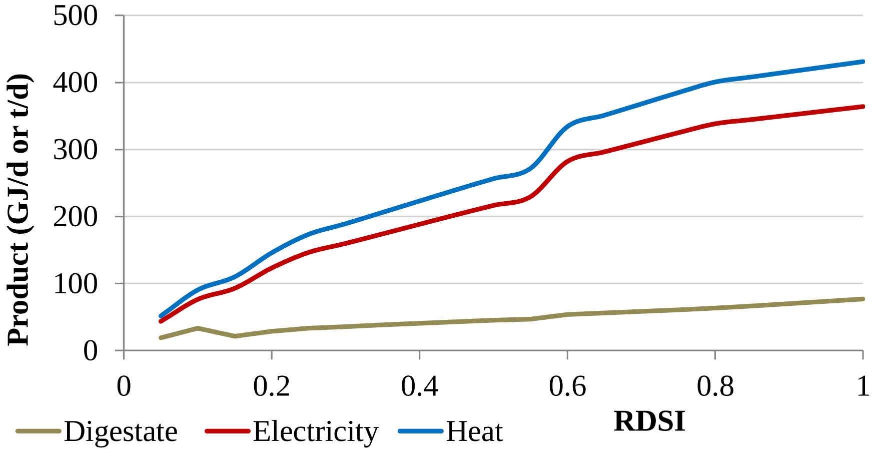


Figure 5-9. Product flow-rate vs. relative direct sustainability index (Kravanja and Čuček, 2013)

Figure 5-10 shows how the product flowrates change with any increasing of the RTSI.

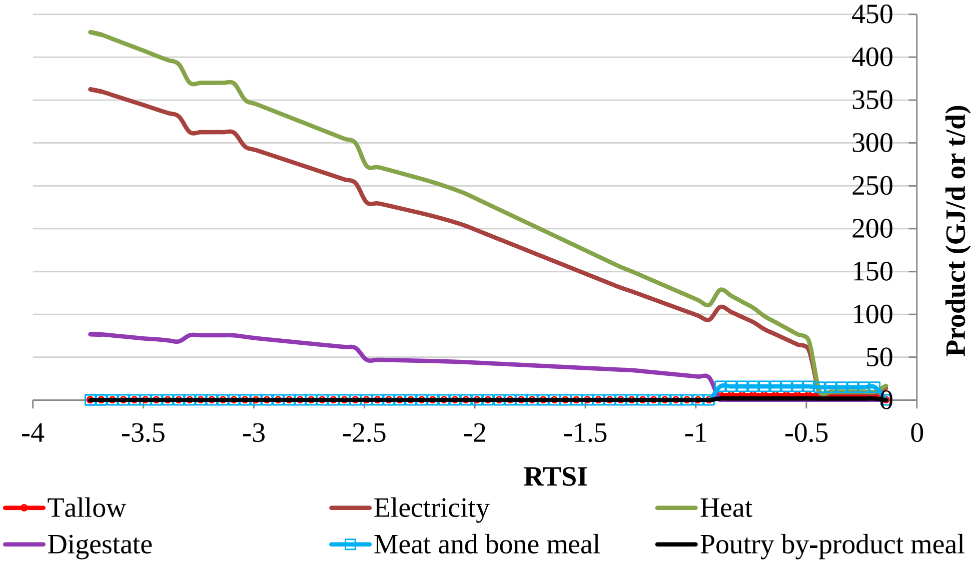


Figure 5-10. Product flow-rate vs. relative total sustainability index (Kravanja and Čuček, 2013)

Only the AD process is selected from throughout the whole range of relative direct sustainability indexes, and the produced products are electricity, heat, and digestate (organic fertiliser). The mass flow-rates of the solid products from the rendering plant (meat, bone and poultry by-product meal) are zero.

Throughout the whole range of relative total sustainability indexes, the AD process is again selected, and within the range of RTSI $-0.9 \leq \text{RTSI} \leq -0.15$ the rendering process is selected for the production of meat, bone, and poultry by-product meal, and tallow. The rendering process is therefore still a sustainable alternative, however much less than the production of biogas from animal and organic wastes. The production of products from AD and the rendering process is shown in Table 5-13 for maximal RDSI and minimal RTSI (and maximal profit – reference value), for the lowest RDSI (RDSI ≈ 0.05) and for the highest RTSI (RTSI ≈ -0.15).

It can be seen from Figure 5-9 and Figure 5-10 that all the products decrease by decreasing the RDSI, and by increasing the RTSI. By decreasing the RDSI and increasing the RTSI to zero, the biogas production is also close to zero, whilst the rendering products are only optimal for the highest values of RTSI.

Table 5-13. Production by the maximal and minimal values of RSI

	RDSI = max, RTSI = min	RDSI = 0.05	RTSI = -0.19
Electricity (GJ/d)	364.13	43.60	8.35
Heat (GJ/d)	431.21	51.64	9.88
Digestate (t/d)	76.83	19.21	0
Meat and bone meal (t/d)	0	0	15.01
Tallow (t/d)	0	0	5.63
Poultry by-product meal (t/d)	0	0	1.76

It can be seen from the results that for the maximal profit the worst and wrong solutions are obtained when considering only the direct effects; and the best and right solutions when also considering the indirect effects, and when comparing with the current situation. It should be noted that in this new approach when considering total effects, the profit and RTSI act at the same time towards improving both the economy and the environment, so that non-trade-off optimal solutions can thus be obtained.

5.3 Concept of Eco- and Total Profit and other Combined Criteria

The aim of this part of the work is the development of sustainable LCA-based MILP synthesis for biogas production and its supply chain, by simultaneously considering two combined dimensions of SD – economic and environmental within the objective function. The innovative concepts of eco-profit, net profit, and total profit are developed in order to assess the environmental impacts. They all use the eco-cost coefficients, as determined in accordance with the LCA (Delft University of Technology, 2012). The analysis includes the production of renewable raw materials, production of bioenergy, its distribution, transportation paths, and waste management. It is applied to an integrated biogas production process with included auxiliary facilities (see Section 5.2.4 and Figure 5-6).

Different criteria are used, such as eco-cost, eco-benefit or eco-revenue, eco-profit, net profit and total profit. The advantages of all these criteria are that they are expressed in monetary value per time unit. In order to define these criteria, different sets are used, R_{B}, R_{UNB}, P_{B}, and P_{UNB}, as defined and used throughout the model for raw materials and products (see Section 5.2):

i) R_{B} – set of those raw materials that only burden the environment if processed.
ii) R_{UNB} – set of those raw materials that also unburden or benefit the environment when used.
iii) P_{B} – set of those products that only burden the environment in relation to processing, disposal, and transportation.
iv) P_{UNB} – set of those products that also unburden or benefit the environment.

5.3.1 Eco-Cost, Eco-Benefit and Eco-Profit

The eco-cost and eco-benefit coefficients have the advantage of being directly incorporated into the objective function, together with a given economic objective. Therefore the LCA practitioner is not exposed to setting subjective weights between sustainability (economic and environmental) objectives, however the subjectivity of this approach is incompletely eliminated.

5.3.1.1 Eco-Cost (Burdening of the Environment)

Eco-cost is an indicator based on LCA and describes environmental burden on the basis of preventing that burden. It is a sum of the marginal prevention costs during the life cycle, the sum of eco-costs of material depletion, eco-costs of energy and transport, and eco-costs of emissions. Eco-costs are those costs that should be made in order to reduce the environmental pollution and material depletion to a level that is in line with the carrying capacity of the Earth (Vogtländer et al., 2010). For example the eco-cost calculation for CO_2 emissions, for each t of CO_2 emission, 135 € should be invested in offshore windmill parks or other CO_2 reduction systems (Vogtländer et al., 2010). Similar calculations can be made for other environmental burdens too, e.g. for acidification or for summer smog. Eco-costs are virtual costs, and are not yet integrated into current prices. They are regarded as hidden obligations (Vogtländer et al., 2010).

The advantages of eco-cost coefficients are (Vogtländer et al., 2010):

i) They are expressed as a monetary value (€/unit);
ii) There is no need to compare two products, processes or services (as is often aimed of LCA);

iii) Calculations are based on current European price levels;

iv) Eco-cost coefficients were updated in 2007, 2010 and 2012 (Delft University of Technology, 2012).

Eco-cost (c^{Eco}) is defined as the sum of all the negative impacts from burdens on the environment, and is defined using Equation (5.10), where instead of I_o^{d}, c^{Eco} is used, instead of specific sustainability indicators ($I_{o,p}^{s}$ and $I_{o,p}^{s,t}$), eco-cost coefficients (c_p^{s} and $c_p^{\text{s,tr}}$) are employed:

$$c^{\text{Eco}} = \sum_{p \in R_{\text{B}} \cup R_{\text{UNB}} \cup P_{\text{B}} \cup P_{\text{UNB}}} q_p^m \cdot c_p^{\text{s}} + \sum_{p \in R_{\text{B}} \cup R_{\text{UNB}} \cup P_{\text{B}} \cup P_{\text{UNB}}} q_p^m \cdot l_p \cdot D_p \cdot c_p^{\text{s,tr}} \tag{5.18}$$

Eco-costs also include burdens originating from the extraction of raw materials, disposal and purification of products, and from all transportation and distribution paths within the supply chain.

5.3.1.2 *Eco-Benefit (Unburdening of the Environment)*

Eco-benefit or eco-revenue (R^{Eco}) represents the unburdening of the environment and is defined as the sum of all the positive impacts of unburdening the environment, similarly to I_o^{ind} – Equation (5.11), where instead of I_o^{ind}, R^{Eco} is used, and instead of specific sustainability indicators ($I_{o,p}^{s}$ and $I_{o,p}^{s,t}$) the eco-benefit coefficients (c_p^{s} and $c_p^{\text{s,tr}}$) are employed:

$$R^{\text{Eco}} = \sum_{p \in R_{\text{UNB}}} q_p^m \cdot c_p^s + \sum_{p \in P_{\text{UNB}}} q_m^p \cdot f_p^{S/P_{\text{UNB}}} \cdot c_p^s \tag{5.19}$$

5.3.1.3 *Eco-Profit (Eco-Benefit – Eco-Cost)*

Annual eco-profit P^{Eco} (€/y) is defined as an analogy with economic profit, as the difference between eco-benefit or eco-revenue in €/y (unburdening) and eco-cost in €/y (burdening):

$$P^{\text{Eco}} = R^{\text{Eco}} - c^{\text{Eco}} \tag{5.20}$$

5.3.2 Net and Total Profit

Net profit (P^{N}) is defined as the economic profit (P^{Econ}) reduced by the eco-cost (c^{Eco}). The synthesis problem, where economic profit and eco-cost are optimised simultaneously, and takes the following form:

$$\begin{aligned}
&P^{\mathrm{N}}(x,y)=\max(P^{\mathrm{Econ}}(x,y)-c^{\mathrm{Eco}}(x,y))\\
&\text{s.t.}\quad h(x,y)=0\\
&\qquad g(x,y)\le 0 \qquad\qquad \text{(Net profit MINLP)}\\
&\qquad (x^{\mathrm{LO}}\le x\le x^{\mathrm{UP}})\in X\subset R^{n},\;\; y\in Y=\{0,1\}^{m}
\end{aligned}$$

Total profit (P^{T}) is the summation of the economic profit (P^{Econ}) and eco-profit (P^{Eco}). In the synthesis problem, where economic profit and eco-profit are optimised simultaneously, the solutions obtained are those with maximal total profit:

$$\begin{aligned}
&P^{\mathrm{T}}(x,y)=\max(P^{\mathrm{Econ}}(x,y)+P^{\mathrm{Eco}}(x,y))\\
&\text{s.t.}\quad h(x,y)=0\\
&\qquad g(x,y)\le 0 \qquad\qquad \text{(Total profit MINLP)}\\
&\qquad (x^{\mathrm{LO}}\le x\le x^{\mathrm{UP}})\in X\subset R^{n},\;\; y\in Y=\{0,1\}^{m}
\end{aligned}$$

5.3.3 Illustrative Example

The presented approach is illustrated through a case study comprised of an integrated biogas production supply chain (see Section 5.2.4). The original linearised MINLP model (Drobež et al., 2010) is extended to include consideration of the eco-profit, net profit and total profit. It comprises a process synthesis model, HI model for fixed temperatures, sets of linking equations between the process synthesis and HI models, an objective function with the piecewise linearisation of non-linear non-convex investment terms, and the LCA evaluation of eco-profit.

5.3.3.1 Input Data

Part of the input data was obtained through the company’s experts, and the data for the assessment of eco-profit were obtained mainly from the web site of (Delft University of Technology, 2012). They are presented in Table 5-14 and Table 5-15 for raw materials and in Table 5-16 and Table 5-17 for the products. Those eco-costs associated with constructing a biogas and rendering plant, and the manufacturing of machinery and with human labour were omitted for reasons of simplification. However, it should be noted, that data on eco-costs are very general, and that it would be necessary to carry out the more detailed definition of eco-cost and eco-benefit coefficients, in order to obtain more precise eco-profit, net profit and total profit solutions. Table 5-14 shows the eco-cost and eco-benefit coefficients of the raw materials and their interpretations.

Table 5-15 shows the eco-costs of raw materials, resulting from their transportation from the locations of the raw material to the location of the biogas and rendering plants. These raw materials are different distances from the plants and different means of transport have to be used. There are two options for transporting water, by cisterns or by pipelines.

Table 5-14. Eco-cost and eco-benefit coefficients for the raw materials

Raw material	Eco-cost coefficient* (€/t)	Eco-benefit coefficient (€/t)	Interpretation
Raw materials that only burden the environment if processed, R_B			
Maize silage	6.4	0	Production of maize silage
Water	3	0	Treatment of polluted water
Raw materials that mainly benefit the environment if processed, R_{UNB}			
IW	0	3	Wastewater treatment is unnecessary
Manure	0	22	There are no GHG emissions and other harmful effects on the environment
Animal offal	0	9	Incineration or disposal is unnecessary
Blood	0	9	Incineration or disposal is unnecessary
Wastes**	0	9	Incineration or disposal is unnecessary
Poultry litter	0	22	There are no GHG emissions and other harmful effects on the environment
Hatchery waste	0	0	/
Grape skins	0	0	/
Flotate	0	5	Incineration or disposal is unnecessary

*Eco-cost coefficients are considered without transportation

**waste from the production of poultry meat

Table 5-15. Eco-costs of raw materials due to their transportation to the plants

Raw material	Location of the raw material	Distance to the plant (km)	Eco-cost coefficient of transport	Transport mean
Maize silage	surroundings of Location 1	5	0.0113 €/(m^3.km)	Tractor with trailer
Water from a local well	near the plant	0	0	/
Grape skins	surroundings of Location 2	20	0.0113 €/(m^3.km)	Tractor with trailer
IW*	Location 2	7	12 €/km	Water network
		10	0.13 €/(t.km)	Tank trailer (cistern)
Manure	Location 1	1	0.13 €/(t.km)	Tank trailer (cistern)
	Location 3	20		
Animal offal	Location 2	10	0.514 €/(t.km)	Truck
	Location 4	140		
Blood	Location 2	10	0.514 €/(t.km)	Truck
	Location 4	140		
Waste**	Location 2	10	0.514 €/(t.km)	Truck
Poultry litter	Location 1	2	0.13 €/(t.km)	Tank trailer (cistern)
Hatchery waste	Location 1	3	0.514 €/(t.km)	Truck
Flotate	Location 2	10	0.514 €/(t.km)	Truck
	Location 4	140		

* the source of IW from the prepared meals factory is 7 km away from the plant, and the source of IW generated in the meat industry is 10 km away from the plant

** waste from the production of poultry meat

Table 5-16 presents the eco-cost and eco-benefit coefficients for the products.

Table 5-16. Eco-cost and eco-benefit coefficients for products and their interpretations

Product	Eco-cost coefficient (€/t)	Eco-benefit coefficient (€/t)	Interpretation
Products that only burden the environment if processed, P_B			
Wastewater	3 €/t	-	Wastewater treatment
Products that mainly benefit the environment if processed, P_{UNB}			
Heat	2 €/GJ	12 €/GJ	Heat from the network is replaced
Electricity	18 €/GJ	26 €/GJ	Electricity from the network is replaced
Organic fertiliser	64 €/t	612 €/t	Inorganic fertilisers are replaced
Meat and bone meal	0.11 €/t	27 €/t	Protein concentrates are replaced
Tallow	0.1 €/t	500 €/t	Palm oil is replaced
Poultry by-product meal	0.11 €/t	27 €/t	Protein concentrates are replaced

Eco-benefits are caused due to the replacement of conventional, mainly non-renewable products, with renewable products. Substitution factors are assumed to be the same, as defined in Table 5-8.

Table 5-17 shows the eco-cost coefficients for those products, caused due to their distribution.

Table 5-17. Eco-costs of products due to their distribution

Product	The distance to the user/disposal (km)	Eco-cost coefficient of distribution	Distribution
Wastewater	10	12 €/km 0.13 €/(t·km)	Water network Tank trailer (cistern)
Heat	5	12 €/km	Water network
Electricity	0.5	10.7 €/m	Distribution network
Organic fertiliser	10	0.13 €/(t·km)	Tank trailer (cistern)
Meat and bone meal	200	0.26 €/(t·km)	Truck
Tallow	200	0.26 €/(t·km)	Truck
Poultry by-product meal	200	0.26 €/(t·km)	Truck

5.3.4 Results from Single-Objective Optimisation

5.3.4.1 Maximisation of an Economic Profit

An economic profit of 3.668 M€/y, an eco-profit of 2.673 M€/y, and total profit of 6.341 M€/y are obtained, where the eco-cost is 5.294 M€/y and net profit -1.626 M€/y. The optimal solution in terms of biogas production includes the use of a thermophilic process that converts the liquid pig manure and other substrates, using no additional process water. The reconstruction of the existing pig farm and a closed water system with ultrafiltration and reverse osmosis are selected. From an economic perspective, it is better to recycle and reuse the process water, because the meat company has to pay for the treatment of process wastewater (2.5 €/t) (see Figure 5-7) within the central treatment unit. The main results obtained by maximisation of the economic profit are shown in Table 5-18.

Table 5-18. Optimal results obtained by SOO

	Maximised economic profit (P)	Minimised eco-cost (c^{Eco})	Maximised eco-profit (P^{Eco})	Maximised net-profit (P^{N})	Maximised total profit (P^{T})
Economic profit (M€/y)	**3.668**	0	1.444	0	3.591
Eco-cost (M€/y	5.294	**0**	2.910	0	4.948
Eco-profit (M€/y)	2.673	0	**3.621**	0	2.929
Net profit (M€/y)	-1.626	0	-1.466	**0**	-1.358
Total profit (M€/y)	6.341	0	5.065	0	**6.520**
Income (M€/y)	7.354	0	6.283	0	7.249
Depreciation (M€/y)	2.943	0	2.526	0	2.925
Investment (M€)	20.727	0	17.786	0	20.600
Operating costs (M€/y)	3.686	0	4.839	0	3.658
Biogas production (m^3/d)	43,281	0	28,267	0	42,623
The amount of used waste (t/y)	122,861	0	116,836	0	121,180
RDSI	1	0	0.726	0	0.989
RTSI	-3.781	0	-2.884	0	-3.725

5.3.4.1 Maximisation of an Eco-Profit

An eco-profit of 3.621 M€/y, an economic profit of 1.444 M€/y and total profit of 5.065 M€/y are obtained. The optimal solution includes the use of a thermophilic process for converting the liquid pig manure and other substrates with no additional water, and the use of a rendering plant converting slaughterhouse waste, bones, and animal offal to meat and bone meal, tallow and poultry by-product meal. Now, an open water system is selected with a central treatment unit. This solution indicates that, from the viewpoint of eco-profit, it is better to prevent the production and use of organic fertiliser. It is required in much larger quantities as inorganic fertiliser for the same effect; a substitution factor of 34 is assumed, however it could be even higher (Caslin, 2009). Therefore, the eco-cost is higher for organic fertiliser compared to inorganic. Also, raw materials far away from the plant (140 km) are deselected because of the considerable eco-cost of transportation. Figure 5-11 presents the optimal biogas production process obtained by the maximisation of eco-profit. The results obtained by maximisation of the eco-profit are shown in Table 5-18.

5.3.4.2 Maximisation of an Net Profit

Maximisation of the net profit corresponds to the maximisation of the economic profit simultaneously with the minimisation of eco-cost. The results obtained by maximisation of the net profit are shown in Table 5-18. It is interesting to note that a zero solution was obtained by the maximisation of net profit because the economic profit was outnumbered by the eco-cost. The solution indicates that it would be better not to operate from the environmental point of view. However, this conclusion is wrong – the production of biogas from waste is certainly sustainable because the use of waste and the production of biogas considerably unburden the environment.

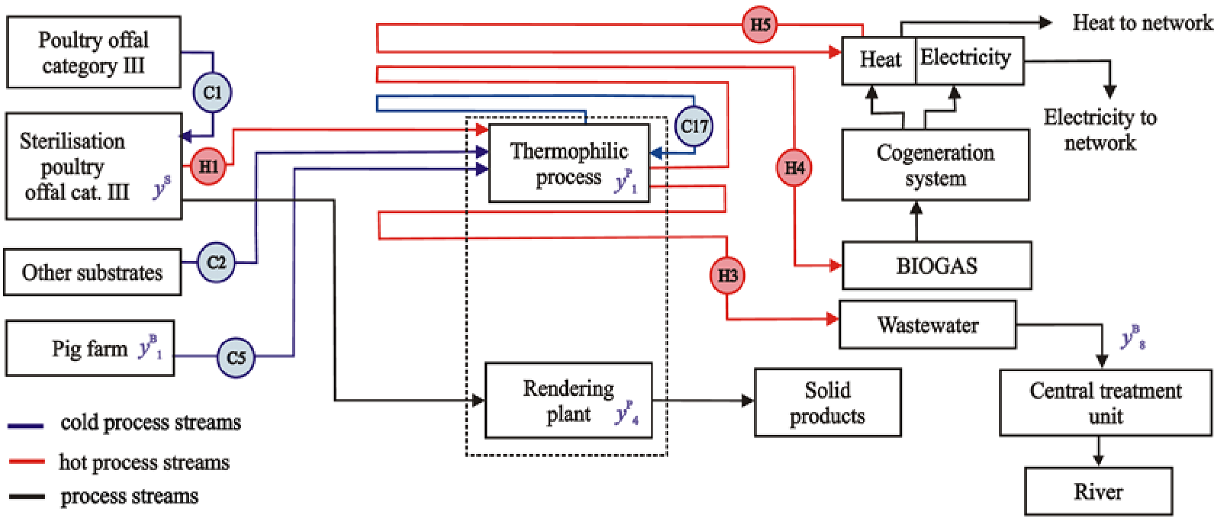


Figure 5-11. Optimal process obtained by maximisation of eco-profit (modified from (Čuček et al., 2012a))

5.3.4.3 Maximisation of an Total Profit

A total profit of 6.520 M€/y is obtained, with 3.591 M€/y of economic and 2.929 M€/y of eco-profit. The optimal process scheme is the same as in the case when maximising economic profit alone (see Figure 5-7). Note that this economic profit is from the maximal one decreases only slightly, from 3.668 M€/y to 3.591 M€/y, whilst the eco-profit, at the same time, is improved much more, from 2.667 M€/y to 2.924 M€/y. This means that investing about 77,000 €/y in pollution prevention would result in about 257,000 €/y eco-savings, and this could be achieved only by rejecting the use of raw materials far away from the plant. Note that the biogas production slightly decreases; from 43,281 m^3/d to 42,623 m^3/d. The solution indicates that the optimal trade-off between biogas production and eco-cost for transportation of raw materials is established at the point of the maximal total profit.

From Table 5-18 it can be seen that by the maximal profit the worst and wrong solutions are obtained when considering only the direct effects; and the best and right solutions when considering also indirect effects and when comparing to the current situation. When considering total effects, the total profit and RTSI act at the same time towards improving both, the economy and the environment so that non-trade-off optimal solutions are thus obtained.

This SOO model consists of approximately 650 constraints, 900 single variables, and 300 binary variables where most of the binary variables are used in the piece-wise linearisation of investment terms. For the solving of MILP problem, the modelling system GAMS and high performance MILP solver CPLEX (IBM, 2012) are used.

5.3.5 Results from Multi-Objective Optimisation

MOO is performed in order to review the relationship between the economic profit and eco-profit regarding wider ranges of economic profit and eco-profit. A set of Pareto optimal solutions is obtained (Figure 5-12) from the maximum economic profit (3.668 M€/y) and minimum eco-profit (2.673 M€/y), where the thermophilic process and closed water system are selected, to a solution with minimum economic profit (1.444 M€/y) and maximum eco-profit (3.621 M€/y), where the thermophilic process with a rendering plant, and open water system are selected. In-between, the economic profit first decreases drastically by 1.006 M€/y, then by 0.554 M€/y, and finally by 0.664 M€/y because of the structural changes, the more important being the use of the rendering process first, then the opening of the water system by rejecting the rendering process, and lastly by again selecting the rendering plant, now with the open water system at the point of the maximum eco-profit.

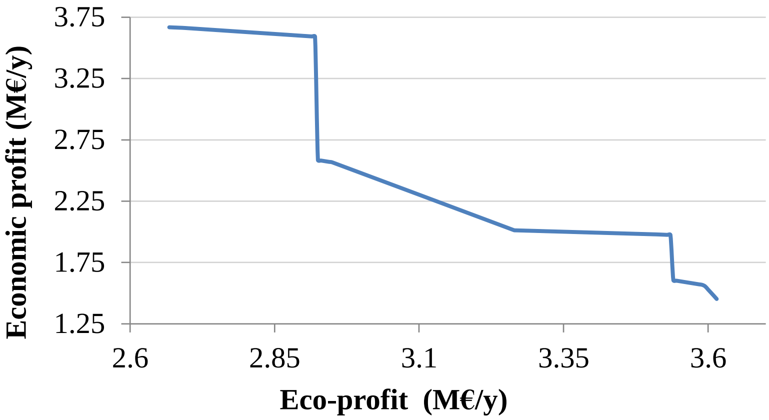


Figure 5-12. Pareto curve showing trade-offs between economic and eco-profit (Čuček et al., 2012a)

From the economic aspect, it is better to re-use the purified process wastewater (closed water system) and to convert the slaughterhouse waste, bones, and animal offal into biogas, whilst from the eco-aspect it is preferable to avoid the production and use of organic fertiliser, to purify the organic fertiliser within the central treatment unit, and to use the rendering plant to convert slaughterhouse waste, bones, and animal offal to meat and bone meal, tallow and poultry by-product meal. It can be seen from Figure 5-12, that all the results from the MOO are positive, for both economic profit and eco-profit, indicating that biogas production from organic waste is an economically-viable and environmentally-sustainable alternative. The most economically-attractive solutions are also environmentally-attractive, and cause an unburdening of the environment. The result obtained by the maximisation of total profit (6.520 M€/y; 3.591 M€/y of economic profit, and 2.929 M€/y of eco-profit) indicates that the appropriate trade-off between economic profit and eco-profit could be obtained.

6 REDUCING THE DIMENSIONALITY OF THE CRITERIA IN MULTI-OBJECTIVE OPTIMISATION

This final Chapter presents the developed novel dimensionality reduction method – a ROM, applied to environmental footprints, by which the number of environmental footprints within the MOO is reduced to a minimum number of representative footprints (Čuček et al., 2013a).

6.1 Representative Objectives Method

The aim of this work is to introduce a methodology (principle and procedure) based on the novel ROM for identifying similarities amongst different objectives (direct environmental footprints) within MOO. The dimensionality reduction at optimisation $k \in K$ by the proposed ROM for objectives $o \in O$, comprised of annual profit P and different environmental footprints $F_{f,k}(x), \forall (f \in FP \wedge k \in K)$, is solved over three main steps: i) generation of solution points for analysing similarities amongst the footprints, ii) identification of similarities amongst the footprints and the selection of representative footprints (those footprints that show similar behaviour are grouped into subsets, each subset's representative footprint is then selected), and iii) the performing of MOO for maximising profit with respect to the representative footprints. In this way, the dimensionality of the criteria within the MOO could be significantly reduced. The remaining footprints are read directly from Pareto solutions. Using this novel approach makes MOO more practical for real life problems. The presented dimensionality reduction method is applicable in those cases when the model is known.

6.1.1 Generation of Points Used for Analysing Similarities amongst Footprints

The environmental footprints $F_{f,k}(x), f \in FP$ are obtained using the following Equation:

$$F_{f,k}(x) = \sum_{v \in V} \mathrm{a}_{f,v} \cdot x_{v,k} \qquad \forall (f \in FP, k \in K) \tag{6.1}$$

where $\mathrm{a}_{f,v}$ are the matrix coefficients (specific environmental footprints), and $x_{v,k}$ are the corresponding process variables at iteration $k \in K$ (see Equations (5.1) – (5.5) in Section 5.1.2). Both, the coefficients and values of the process variables are used for the calculating of different measurements when identifying similarities amongst footprints. As the measurements should reflect the obtaining of maximal profits at various values of footprints, the multi-criteria approach should be applied along the whole range of footprints.

The footprints at optimisation iteration k are normalised in order to adjust their values to a common scale. Relative footprints $(F^{r}_{f,k}(x))$ are obtained in this way – see Equation (5.9). In order to keep the problem at a manageable level, 2-D MOO is applied – see $(\mathrm{MINLP}-2)_{f,k}, \forall f \in FP$ in Section 5.1.2.5, where all the footprints are simultaneously forced to decrease sequentially from their maximal values until there is no feasible solution. $|K|$ Pareto optimal solutions x_k are obtained in terms of the overall environmental burden. As all the footprints are simultaneously constrained, the solutions are located below all footprint-individual Pareto curves.

6.1.2 Identifications of Similarities amongst Footprints

Three partitioning criteria for identifying similarities amongst footprints are proposed:

i) Normalised ratios between pairs of footprints (f and ff) for selected optimal point x_k :

$$R_{f,ff,k} = \sum_{v \in V, \mathrm{a}_{ff,v} \neq 0} \left(\frac{\dfrac{\mathrm{a}_{f,v}}{\mathrm{a}_{ff,v}}}{\dfrac{F_{f,k}}{F_{ff,k}}} \cdot \frac{\mathrm{a}_{f,v} \cdot x_{v,k}}{F_{f,k}} \right) \qquad \forall (f \in FP, ff \in FP, k \in K) \tag{6.2}$$

Because $R_{f,ff,k}$ can differ from $R_{ff,f,k}$, the geometric mean is calculated:

$$GR_{f,ff,k} = \sqrt{R_{f,ff,k} \cdot R_{ff,f,k}} \qquad \forall (f \in FP, ff \in FP, k \in K) \tag{6.3}$$

and then the mean values for the generated points are finally obtained, which are calculated as the ratios between pairs of footprints (and its geometric mean) divided by the number of iterations k (cardinality of a set K):

$$R^{\mathrm{m}}_{f,ff} = \frac{\sum_{k \in K} R_{f,ff,k}}{|K|} \qquad \forall (f \in FP, ff \in FP) \tag{6.4}$$

$$GR^{\mathrm{m}}_{f,ff} = \frac{\sum_{k \in K} GR_{f,ff,k}}{|K|} \qquad \forall (f \in FP, ff \in FP) \tag{6.5}$$

Note, that geometric means are applied in order that smaller normalised ratios contribute more than larger values. For perfect similarity, the normalised ratio between pairs of footprints is 1.

ii) Overlapping pairs of footprints (f and ff) within the process variables for the selected optimal point x_k :

$$O_{f,ff,k} = \sum_{v \in V, \mathrm{a}_{f,v} \neq 0 \wedge \mathrm{a}_{ff,v} \neq 0} \frac{\mathrm{a}_{f,v} \cdot x_{v,k}}{F_{f,k}} \qquad \forall (f \in FP, ff \in FP, k \in K) \tag{6.6}$$

Because $O_{f,ff,k}$ can be different from $O_{ff,f,k}$, the geometric mean is calculated as:

$$GO_{f,ff,k} = \sqrt{O_{f,ff,k} \cdot O_{ff,f,k}} \qquad \forall (f \in FP, ff \in FP) \tag{6.7}$$

The mean values than are:

$$O^{\mathrm{m}}_{f,ff} = \frac{\sum_{k \in K} O_{f,ff,k}}{|K|} \qquad \forall (f \in FP, ff \in FP), \text{ and} \tag{6.8}$$

$$GO^{\mathrm{m}}_{f,ff} = \frac{\sum_{k \in K} GO_{f,ff,k}}{|K|} \qquad \forall (f \in FP, ff \in FP) \tag{6.9}$$

If footprint f is defined for the same process variables as footprint ff, then the overlap coefficient is 1.

iii) Average absolute normalised deviation between pairs of footprints $(f$ and $ff)$ for selected optimal point x_k :

$$D_{f,ff,k} = \frac{\sum_{v \in V, \mathrm{a}_{ff,v} \neq 0} \left(\left| \frac{1 - \frac{\mathrm{a}_{f,v}}{\mathrm{a}_{ff,v}}}{\frac{F_{f,k}}{F_{ff,k}}} \cdot \frac{\mathrm{a}_{f,v} \cdot x_{v,k}}{F_{f,k}} \right| \right))}{(\sum_{v \in V, \mathrm{a}_{ff,v} \neq 0} 1) - 1} \qquad \forall (f \in FP, ff \in FP, k \in K) \tag{6.10}$$

Small values of $D_{f,ff}$ indicating good agreement between pairs of footprints. Now, smaller values should contribute as equally as the larger values. The arithmetic mean is thus calculated between $D_{f,ff}$ and $D_{ff,f}$:

$$AD_{f,ff,k} = \left(D_{f,ff,k} + D_{ff,f,k} \right) / 2 \qquad \forall (f \in FP, ff \in FP, k \in K) \tag{6.11}$$

Finally, their mean values for the generated points are:

$$D^{\mathrm{m}}_{f,ff} = \frac{\sum\limits_{k\in K} D_{f,ff,k}}{|K|} \qquad \forall (f \in FP,\ ff \in FP) \tag{6.12}$$

$$AD^{\mathrm{m}}_{f,ff} = \frac{\sum\limits_{k\in K} AD_{f,ff,k}}{|K|} \qquad \forall (f \in FP,\ ff \in FP) \tag{6.13}$$

Based on the values of the above partitioning criteria, footprints $f \in FP$ are partitioned into N_{S} subsets $s \in S$ of similar footprints $fs_s \in FS_s$, each subset being composed of one representative footprint $fr_s \in FS_s^{fr}$ and the remaining unrepresentative footprints $fu_s \in FS_s^{fu}$; $FS_s^{fr} \cup FS_s^{fu} = FS_s$. Thus, N_{S} representative footprints $fr_s,\ s \in S$ are identified (ideally two or three). In given subsets, those footprints are selected that have normalised ratios close to one. Overlap values and average absolute normalised deviations have to be checked if they are close to 1 and 0. One representative footprint is selected from amongst footprints within a given subset, either based on their priority or their overlap values. In a situation where the above criteria do not yield the sufficient and desirable similarities amongst the footprints, more subsets with more representative footprints should be selected, up to the number of evaluated footprints.

6.1.3 Multi-Objective Optimisation

In the last step, a MOO is performed for N_s selected representative footprints, $fr_s,\ s \in S$, where the main criterion is the maximisation of the profit. The following $(\mathrm{MI(N)LP})_{k_1,\dots,k_{N_{\mathrm{S}}}}$ $(\mathrm{MI(N)LP})_{k_1,\dots,k_{N_{\mathrm{S}}}}$ problem is defined as:

$$\begin{aligned}
&\max_{x,y}\ P_{k_1,\dots,k_{N_{\mathrm{S}}}} = c^{\mathrm{T}} y + f(x) - \sum_{f\in FP} w \cdot F_{f,k}(x) \\
&\text{s.t.} \qquad Ay + h(x,y) = 0 \\
&\qquad\qquad By + g(x,y) \le 0 \\
&\qquad\qquad F^{r}_{fr_s,k_s}(x) \le \varepsilon_{s,k_s}, \qquad \forall fr_s \in FS_s^{fr},\ s \in S \\
&\qquad\qquad (x^{\mathrm{LO}} \le x \le x^{\mathrm{UP}}) \in X \subset R^n,\ \ y \in Y = \{0,1\}^m
\end{aligned} \qquad (\mathrm{MI(N)LP})_{k_1,\dots,k_{N_{\mathrm{S}}}}$$

The ε-constraint method is applied to this MOO problem, with representative footprints being the varying parameters within the loops. The sequences of single-objective $(\mathrm{MI(N)LP})_{k_1,\dots,k_{N_{\mathrm{S}}}}$ $(\mathrm{MI(N)LP})_{k_1,\dots,k_{N_{\mathrm{S}}}}$ problems are thus solved for representative footprints as the maximisation of the profit subjected to these relative representative footprints. N_{S}-embedded loop statements are used to repeatedly solve the $(\mathrm{MI(N)LP})_{k_1,\dots,k_{N_{\mathrm{S}}}}$ $(\mathrm{MI(N)LP})_{k_1,\dots,k_{N_{\mathrm{S}}}}$ problem, where during the sequence of MI(N)LPs each representative footprint $fr_s, s \in S$ is forced to decrease sequentially from its maximal value $(\varepsilon_s = 1)$ by its suitable step-size $\Delta\varepsilon_s$ until there is no feasible solution:

$$\varepsilon_{1,k_S-1} = \varepsilon_{1,k_S} - \Delta\varepsilon_1, .., (\varepsilon_{N_S,k_S-1} = \varepsilon_{N_S,k_S} - \Delta\varepsilon_{N_S},\ k_{N_S} \in K_{N_S}), .., k_s \in K_s \tag{6.14}$$

A finer Pareto front is obtained when $\Delta\varepsilon_s$ are smaller, e.g. 1 %. A N_s-D, mostly 3-D graph of Pareto optimal solutions is thus obtained. The number of optimisation runs depends on the number of representative footprints and step-sizes $\Delta\varepsilon_s$, and is equal to $\prod_{s \in S}(|K_s|)$; e.g., for two representative footprints and a selected $\Delta\varepsilon_s$ of 1 %, the number of required optimisation runs $k \in K$ is about 10,000.

The remaining footprints can be read directly from the MOO solutions and can be presented together with the selected representative footprints on the plots. In this way the exact solutions are obtained, and any errors associated with the calculations of ‘dependent’ footprints from their correlations with the ‘independent’ ones, are thus avoided.

Two scenarios are then considered with respect to handling the remaining non-representative footprints. In the first one, as in the $(\text{MI(N)LP})_{k_1,...,k_{N_S}}$ $(\text{MI(N)LP})_{k_1,...,k_{N_S}}$ problem, the remaining footprints are unconstrained during the MOO, thus giving rise to more relaxed Pareto solutions in terms of environmental burdens and profit (optimistic solutions). In the second constrained scenario, the whole subset of footprints FS_s^{C} is now simultaneously constrained to the same ε_s (Equation (6.15)), and to the corresponding values obtained at the relaxed optimistic scenario, FS_s^{R} (Equation (6.16)):

$$F_{fs_S,k_S}^{r,\text{C}}(x) \le \varepsilon_{s,k_S}, \qquad \forall(fs_s \in FS_s,\ s \in S) \tag{6.15}$$

$$F_{fs_S,k_S}^{r,\text{C}}(x) \le F_{fs_S,k_S}^{r,\text{R}}, \qquad \forall(fs_s \in FS_s,\ s \in S) \tag{6.16}$$

In this way, the footprints of the second scenario never exceed those of the first scenario.

More rigid Pareto solutions in terms of profit and environmental burdens are thus obtained (pessimistic solutions). Which option to select depends on the decision-makers, either moderated or restricted towards the environment. Both optimistic and pessimistic scenarios were applied within the demonstrated case study.

When footprints grouped within the same subsets are completely correlated, the optimistic and pessimistic solutions are the same, and the error of the dimensionality reduction is zero. If, however, they differ, their difference can be used as a measurement of the error of this

MOO approach. When presenting optimistic solutions, a percentage deviation $\delta_{o,k}^{\mathrm{R}}$ at iteration k for the optimistic value of objective o_k^{R} obtained for the remaining relaxed footprints, with respect to the corresponding pessimistic value o_k^{C} obtained for constrained remaining footprints, is defined for non-zero feasible objectives as follows:

$$\delta_{o,k}^{\mathrm{R}} = \frac{o_k^{\mathrm{R}} - o_k^{\mathrm{C}}}{o_k^{\mathrm{C}}}, \qquad \forall (k \in K, o \in O, o_k^{\mathrm{R}} \neq 0, o_k^{\mathrm{C}} \neq 0) \tag{6.17}$$

The deviations $\delta_{o,k}^{\mathrm{C}}$ associated with pessimistic constrained solutions with respect to the corresponding optimistic relaxed solutions are similarly defined as:

$$\delta_{o,k}^{\mathrm{C}} = \frac{o_k^{\mathrm{C}} - o_k^{\mathrm{R}}}{o_k^{\mathrm{R}}}, \qquad \forall (k \in K, o \in O, o_k^{\mathrm{R}} \neq 0, o_k^{\mathrm{C}} \neq 0) \tag{6.18}$$

Finally, the means of errors are calculated using Equation (6.19) for optimistic relaxed solutions and by using Equation (6.20) for pessimistic constrained solutions for each feasible objective:

$$\mu_o^{\mathrm{R}} = \frac{\sum\limits_{k \in K, o_k^{\mathrm{R}} \neq 0, o_k^{\mathrm{C}} \neq 0} \delta_{o,k}^{\mathrm{R}}}{N_k} \qquad \forall o \in O \tag{6.19}$$

$$\mu_o^{\mathrm{C}} = \frac{\sum\limits_{k \in K, o_k^{\mathrm{R}} \neq 0, o_k^{\mathrm{C}} \neq 0} \delta_{o,k}^{\mathrm{C}}}{N_k} \qquad \forall o \in O \tag{6.20}$$

where N_{K} is the total number of obtained feasible solutions from iterations K $(N_{\mathrm{K}} = \sum\limits_{k \in K, o_k^{\mathrm{R}} \neq 0, o_k^{\mathrm{C}} \neq 0} 1)$. Standard deviation is calculated using Equations (6.21) for relaxed and Equation (6.22) for constrained solutions regarding each feasible objective:

$$\sigma_o^{\mathrm{R}} = \sqrt{\frac{\sum\limits_{k \in K, o_k^{\mathrm{R}} \neq 0, o_k^{\mathrm{C}} \neq 0} (\delta_{o,k}^{\mathrm{R}} - \mu_o^{\mathrm{R}})^2}{N_k - 1}} \qquad \forall o \in O \tag{6.21}$$

$$\sigma_o^{\mathrm{C}} = \sqrt{\frac{\sum\limits_{k \in K, o_k^{\mathrm{R}} \neq 0, o_k^{\mathrm{C}} \neq 0} (\delta_{o,k}^{\mathrm{C}} - \mu_o^{\mathrm{C}})^2}{N_k - 1}} \qquad \forall o \in O \tag{6.22}$$

6.2 Illustrative Example

The simple methodology described above is applied within the case study of regional biomass and bioenergy supply-chains (Čuček et al., 2010) – see Section 4.1, extended for simultaneous assessment of footprints (Čuček et al., 2012e) – see Section 5.1. The MILP synthesis model is solved within MOO by maximising profit as the main objective, while the footprints are constrained by ε when applying the ε-constraint method.

6.2.1 Selection of Points used for Obtaining Similarities amongst the Footprints

Identifications of similarities amongst footprints are performed directly from the matrix of process variables and footprints. The matrix coefficients are shown in Table 6-1.

The matrix coefficients (specific environmental footprints) in Table 6-1 represent:

- $ei^{\mathrm{L1}}_{f,pi}$, $pi \in PI$, $PI = \{\text{corn grain, corn stover, manure, wood chips, MSW, timber}\}$;
- $ei^{\mathrm{L2}}_{f,pi}$, $pi \in PI$, $PI = \{\text{corn grain, corn stover, timber}\}$;
- $ei^{\mathrm{L3}}_{f,pi,t}$, $(pi,t) \in PT$, $PT = \left\{\begin{array}{l}\text{(corn grain, DGP), (wood chips, incineration),}\\ \text{(corn stover, incineration), (MSW,}\\ \text{MSW incineration), (wood chips, MSW}\\ \text{incineration), (corn stover, MSW incineration),}\\ \text{(corn stover, AD), (manure, AD), (timber, sawing)}\end{array}\right\}$;

$ei^{\mathrm{L4}}_{f,p}$, $p \in P$, $P = \{\text{corn grain, heat, electricity, ethanol, board, digestate, DDGS}\}$;

$ei^{\mathrm{tr,L1,L2}}_{f,pi}$, $pi \in PI$, $PI = \{\text{corn grain, corn stover, wood chips, MSW, manure, timber}\}$;

- $ei^{\mathrm{tr,L2,L3}}_{f,pi}$, $pi \in PI$, $PI = \{\text{corn grain, wood chips, MSW, corn stover, manure, timber}\}$;
- $ei^{\mathrm{tr,L2,L4}}_{f,pd}$, $pd \in PD$, $PD = \{\text{corn grain}\}$;
- $ei^{\mathrm{tr,L3,L4}}_{f,pp}$, $pp \in PP$, $PP = \{\text{heat, electricity, ethanol, board, digestate, DDGS}\}$.

Table 6-1. Matrix coefficients for the illustrative example

Matrix coefficient ($a_{f,v}$) / Footprint	CF ($kg/(t\cdot km^2)$)	WF ($kg/(t\cdot km^2)$)	EF ($MJ/(t\cdot km^2)$)	WPF ($kg/(t\cdot km^2)$)	LF ($km^2/t\cdot km^2$)
$ei^{L1}_{f,\text{corn grain}}$	0.154	900	1.726	0.032	$1.37\cdot 10^{-6}$
$ei^{L1}_{f,\text{corn stover}}$	0.154	900	1.726	0.032	0
$ei^{L1}_{f,\text{manure}}$	0	0.75	0	0	0
$ei^{L1}_{f,\text{wood chips}}$	0.066	2,500	0.75	0	0
$ei^{L1}_{f,\text{MSW}}$	0	0.229	0	0	0
$ei^{L1}_{f,\text{timber}}$	0.044	1,500	0.5	0	0
$ei^{L2}_{f,\text{corn grain}}$	0.09	0.5	1.251	0	0
$ei^{L2}_{f,\text{corn stover}}$	0.00262	0.005	0.01504	0	0
$ei^{L2}_{f,\text{timber}}$	0.00078	0.004	0.0108	0	0
$ei^{L3}_{f,\text{corn grain, DGP}}$	0.147	1.3	2.5	0	0
$ei^{L3}_{f,\text{wood chips, incineration}}$	0	0	0	0	0
$ei^{L3}_{f,\text{corn stover, incineration}}$	0	0	0	0	0
$ei^{L3}_{f,\text{MSW, MSW incineration}}$	0.415	0.31	0	0.0016	0
$ei^{L3}_{f,\text{wood chips, MSW incineration}}$	0	0	0	0	0
$ei^{L3}_{f,\text{corn stover, MSW incineration}}$	0	0	0	0	0
$ei^{L3}_{f,\text{corn stover, AD}}$	0	0.091	0	0	0
$ei^{L3}_{f,\text{manure, AD}}$	0	0.091	0	0	0
$ei^{L3}_{f,\text{timber, timber sawing}}$	0.00125	10.6	0.036	0	0
$ei^{L4}_{f,\text{corn grain}}$	0	0	0	0	0
$ei^{L4}_{f,\text{heat}}$	0	0	0	0	0
$ei^{L4}_{f,\text{electricity}}$	0	0	0	0	0
$ei^{L4}_{f,\text{ethanol}}$	0	0	0	0	0
$ei^{L4}_{f,\text{board}}$	0	0	0	0	0
$ei^{L4}_{f,\text{digestate}}$	0.017	0	0	0.00201	0
$ei^{L4}_{f,\text{DDGS}}$	0	0	0	0	0
Matrix coefficient ($a_{f,v}$) / Footprint	CF* ($kg/(t\cdot km^3)$)	WF ($kg/(t\cdot km^3)$)	EF ($MJ/(t\cdot km^3)$)	WPF ($kg/(t\cdot km^3)$)	LF ($km^2/(t\cdot km^3)$)
$ei^{tr,L1,L2}_{f,\text{corn grain}}$	0.000053	0.000136	0.000389	0	0
$ei^{tr,L1,L2}_{f,\text{wood chips}}$	0.00024	0.00049	0.0014	0	0
$ei^{tr,L1,L2}_{f,\text{MSW}}$	0.00013	0.00056	0.0016	0	0
$ei^{tr,L1,L2}_{f,\text{corn stover}}$	0.0011	0.00233	0.00667	0	0
$ei^{tr,L1,L2}_{f,\text{manure}}$	0.000053	0.0001	0.00028	0	0

Table 6-1. Matrix coefficients for the illustrative example (continuation)

Matrix coefficient ($a_{f,v}$) / Footprint	CF* (kg/(t·km^3))	WF (kg/(t·km^3))	EF (MJ/(t·km^3))	WPF (kg/(t·km^3))	LF (km2/(t·km^3))
$ei^{\text{tr,L1,L2}}_{f,\text{timber}}$	0.000053	0.000245	0.0007	0	0
$ei^{\text{tr,L2,L3}}_{f,\text{corn grain}}$	0.000008	0.000073	0.000208	0	0
$ei^{\text{tr,L2,L3}}_{f,\text{wood chips}}$	0.000008	0.000263	0.00075	0	0
$ei^{\text{tr,L2,L3}}_{f,\text{MSW}}$	0.00013	0.00056	0.0016	0	0
$ei^{\text{tr,L2,L3}}_{f,\text{corn stover}}$	0.000008	0.00125	0.00357	0	0
$ei^{\text{tr,L2,L3}}_{f,\text{manure}}$	0.000053	0.0001	0.00028	0	0
$ei^{\text{tr,L2,L3}}_{f,\text{timber}}$	0.000008	0.000131	0.000375	0	0
$ei^{\text{tr,L2,L4}}_{f,\text{corn grain}}$	0.00001	0.00008	0.000264	0	0
$ei^{\text{tr,L3,L4}}_{f,\text{heat}}$	0	0	0	0	0
$ei^{\text{tr,L3,L4}}_{f,\text{electricity}}$	0	0	0	0	0
$ei^{\text{tr,L3,L4}}_{f,\text{ethanol}}$	0.000027	0.000124	0.00035	0	0
$ei^{\text{tr,L3,L4}}_{f,\text{board}}$	0.000008	0.000131	0.000375	0	0
$ei^{\text{tr,L3,L4}}_{f,\text{digestate}}$	0.000053	0.0001	0.00028	0	0
$ei^{\text{tr,L3,L4}}_{f,\text{DDGS}}$	0.000053	0.0001	0.00028	0	0

*CF of rail transport varies significantly depending on the traction, diesel, electric, or diesel-electric traction. CF from electricity production varies considerably between countries according to the share of power plant technologies used. For this reason, and because in the previous reference by authors (Čuček et al., 2010) all biomass and bioproducts had the same values for CF, also here the same values for CF have been assumed. More or less European average conditions are considered (Spielmann et al., 2007).

Firstly, a maximisation of profit using relaxed footprint constraints is carried out. The solution obtained corresponds to the one with maximal footprints. Those maximal values are set as reference footprints F_f^0 and when normalised, relative footprints $F_{f,k}^r$ are obtained and set to 1. The problem $(\text{MINLP}-2)_{f,k}, \forall f \in FP$ introduced in Section 5.1.2.5 is then applied in order to generate those Pareto solutions (green curve in Figure 6-1) used for analysing similarities amongst the footprints. Then the corresponding variables $x_{v,k}$ are selected at the optimal values of the footprints when maximising the profit. In order to present the solution more easily at a smaller size, only several points along the Pareto curves are selected, namely at $F_{f,k}^r$ = 1, 0.8, 0.6, 0.4 and 0.2. Note that all the values at $F_{f,k}^r$ = 0 are 0. The selected Pareto solutions are presented in Table 6-2. The individual footprints' Pareto curves are also presented in Figure 6-1. As expected, they are all located above the green curve.

The environmental footprints could be calculated using Equation (6.1) by applying data from Table 6-1 and Table 6-2. The environmental footprints obtained at the selected Pareto points are presented in Table 6-3. Note that the values obtained at $F^{r}_{f,k}$ = 1, are the reference footprints F^{0}_{f}.

The model formulated as an MILP within GAMS consists of 632 equations, 1,064 single variables and 21 binary variables. Its single-objective problem is solvable in a fraction of a second by MILP solver CPLEX. It should be noted that, as this model was defined as an MILP, and is applied without any optimality gap, the obtained solutions are globally-optimal.

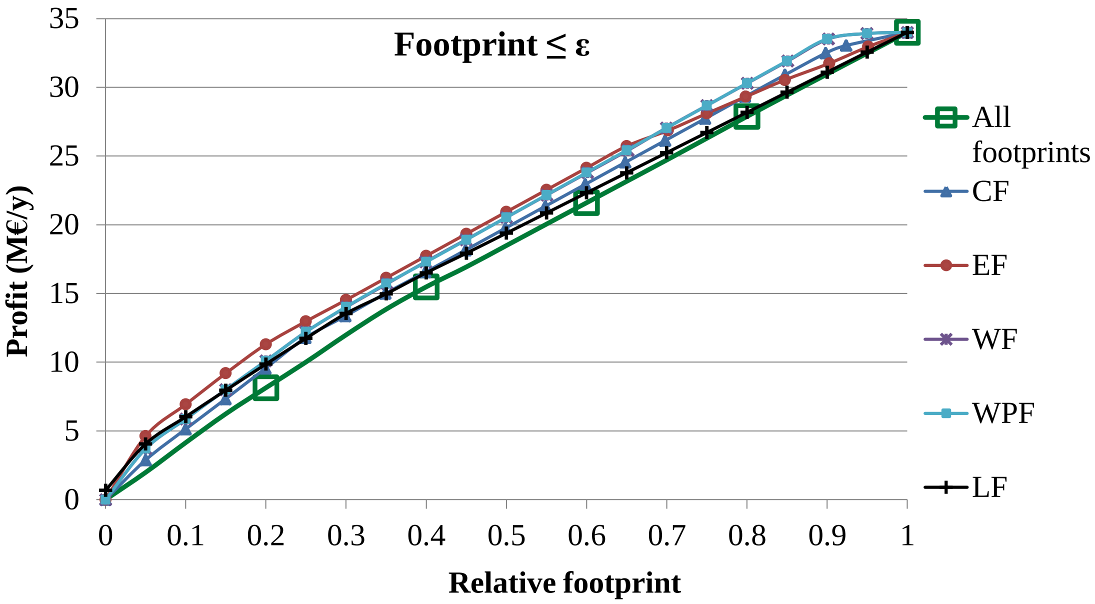


Figure 6-1. Profit vs. direct specific relative footprints (Čuček et al., 2013a)

Table 6-2. Process variables at selected Pareto solutions

Process variable ($x_{v,k}$)/ Footprints at $F^{r}_{f,k}$	1.0	0.8	0.6	0.4	0.2
$\sum_{i\in I} q^{m,\mathrm{L1}}_{i,\text{corn grain}}$, t/y	$2.34\cdot10^{5}$	$1.87\cdot10^{5}$	$1.40\cdot10^{5}$	$9.34\cdot10^{4}$	$4.67\cdot10^{4}$
$\sum_{i\in I} q^{m,\mathrm{L1}}_{i,\text{corn stover}}$, t/y	$1.41\cdot10^{5}$	$1.13\cdot10^{5}$	$8.44\cdot10^{4}$	$5.63\cdot10^{4}$	$2.82\cdot10^{4}$
$\sum_{i\in I} q^{m,\mathrm{L1}}_{i,\text{manure}}$, t/y	$7.30\cdot10^{3}$	0	0	$7.30\cdot10^{3}$	$7.30\cdot10^{3}$
$\sum_{i\in I} q^{m,\mathrm{L1}}_{i,\text{wood chips}}$, t/y	$2.21\cdot10^{3}$	$2.21\cdot10^{3}$	$2.21\cdot10^{3}$	$2.21\cdot10^{3}$	$2.21\cdot10^{3}$
$\sum_{i\in I} q^{m,\mathrm{L1}}_{i,\text{MSW}}$, t/y	$2.12\cdot10^{4}$	$2.12\cdot10^{4}$	$1.65\cdot10^{4}$	0	0
$\sum_{i\in I} q^{m,\mathrm{L1}}_{i,\text{timber}}$, t/y	$2.21\cdot10^{4}$	0	0	$6.64\cdot10^{3}$	0
$\sum_{i\in I}\sum_{m\in M} q^{m,\mathrm{L1,L2}}_{i,m,\text{corn grain}}$, t/y	$2.34\cdot10^{5}$	$1.87\cdot10^{5}$	$1.40\cdot10^{5}$	$9.34\cdot10^{4}$	$4.67\cdot10^{4}$
$\sum_{i\in I}\sum_{m\in M} q^{m,\mathrm{L1,L2}}_{i,m,\text{corn stover}}$, t/y	$1.41\cdot10^{5}$	$1.13\cdot10^{5}$	$8.45\cdot10^{4}$	$5.63\cdot10^{4}$	$2.82\cdot10^{4}$
$\sum_{i\in I}\sum_{m\in M} q^{m,\mathrm{L1,L2}}_{i,m,\text{timber}}$, t/y	$2.21\cdot10^{4}$	0	0	$6.64\cdot10^{3}$	0
$\sum_{n\in N}\sum_{(\text{corn grain, DGP})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{corn grain, DGP}}$, t/y	$1.92\cdot10^{5}$	$1.49\cdot10^{5}$	$1.10\cdot10^{5}$	$7.70\cdot10^{4}$	$3.85\cdot10^{4}$
$\sum_{n\in N}\sum_{(\text{wood chips, incineration})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{wood chips, incineration}}$, t/y	$2.65\cdot10^{3}$	$2.65\cdot10^{3}$	$2.65\cdot10^{3}$	$2.65\cdot10^{3}$	$2.65\cdot10^{3}$
$\sum_{n\in N}\sum_{(\text{corn stover, incineration})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{corn stover, incineration}}$, t/y	$1.39\cdot10^{5}$	$1.13\cdot10^{5}$	$8.44\cdot10^{4}$	$5.45\cdot10^{4}$	$2.63\cdot10^{4}$
$\sum_{n\in N}\sum_{(\text{MSW,MSW incineration})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{MSW,MSW incineration}}$, t/y	$2.12\cdot10^{4}$	$2.12\cdot10^{4}$	$1.65\cdot10^{4}$	0	0
$\sum_{n\in N}\sum_{(\text{wood chips,MSW incineration})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{wood chips,MSW incineration}}$, t/y	0	0	0	0	0
$\sum_{n\in N}\sum_{(\text{corn stover,MSW incineration})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{corn stover,MSW incineration}}$, t/y	0	0	0	0	0
$\sum_{n\in N}\sum_{(\text{corn stover, AD})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{corn stover, AD}}$, t/y	$1.83\cdot10^{3}$	0	0	$1.83\cdot10^{3}$	$1.83\cdot10^{3}$
$\sum_{n\in N}\sum_{(\text{manure, AD})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{manure, AD}}$, t/y	$7.30\cdot10^{3}$	0	0	$7.30\cdot10^{3}$	$7.30\cdot10^{3}$
$\sum_{n\in N}\sum_{(\text{timber, sawing})\in PT} q^{m,\mathrm{T,L2,L3}}_{n,\text{timber, sawing}}$, t/y	$1.77\cdot10^{4}$	0	0	$5.31\cdot10^{3}$	0
$\sum_{m\in M}\sum_{j\in J} q^{m,\mathrm{L2,L4}}_{n,j,\text{corn grain}}$, t/y	0	$5.52\cdot10^{3}$	$5.80\cdot10^{3}$	0	0
$\sum_{n\in N}\sum_{j\in J} q^{m,\mathrm{L3,L4}}_{n,j,\text{heat}}$, MJ/y	$1.25\cdot10^{9}$	$1.02\cdot10^{9}$	$7.71\cdot10^{8}$	$4.79\cdot10^{8}$	$2.54\cdot10^{8}$
$\sum_{n\in N}\sum_{j\in J} q^{m,\mathrm{L3,L4}}_{n,j,\text{electricity}}$, MWh/y	$2.43\cdot10^{5}$	$1.97\cdot10^{5}$	$1.50\cdot10^{5}$	$9.29\cdot10^{4}$	$4.92\cdot10^{4}$
$\sum_{n\in N}\sum_{j\in J} q^{m,\mathrm{L3,L4}}_{n,j,\text{ethanol}}$, t/y	$6.22\cdot10^{4}$	$4.79\cdot10^{4}$	$3.54\cdot10^{4}$	$2.48\cdot10^{4}$	$1.24\cdot10^{4}$
$\sum_{n\in N}\sum_{j\in J} q^{m,\mathrm{L3,L4}}_{n,j,\text{board}}$, t/y	$9.50\cdot10^{3}$	0	0	$2.86\cdot10^{3}$	0

Table 6-2. Process variables at selected Pareto solutions (continuation)

Process variable ($x_{v,k}$)/ Footprints at $F^{r}_{f,k}$	1.0	0.8	0.6	0.4	0.2
$\sum_{n\in N}\sum_{j\in J} q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{digestate}}$, t/y	$3.65\cdot10^{3}$	0	0	$3.65\cdot10^{3}$	$3.65\cdot10^{3}$
$\sum_{n\in N}\sum_{j\in J} q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{DDGS}}$, t/y	$4.81\cdot10^{4}$	$3.72\cdot10^{4}$	$2.74\cdot10^{4}$	$1.92\cdot10^{4}$	$9.62\cdot10^{3}$
$\sum_{i\in I}\sum_{m\in M} D^{\mathrm{L1,L2}}_{i,m}\cdot f^{\mathrm{road,L1,L2}}_{i,m}\cdot q^{m,\mathrm{L1,L2}}_{i,m,\mathrm{corn\ grain}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.50\cdot10^{6}$	$1.10\cdot10^{6}$	$7.58\cdot10^{5}$	$5.16\cdot10^{5}$	$2.21\cdot10^{5}$
$\sum_{i\in I}\sum_{m\in M} D^{\mathrm{L1,L2}}_{i,m}\cdot f^{\mathrm{road,L1,L2}}_{i,m}\cdot q^{m,\mathrm{L1,L2}}_{i,m,\mathrm{wood\ chips}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$2.14\cdot10^{4}$	$2.14\cdot10^{4}$	$3.03\cdot10^{4}$	$2.14\cdot10^{4}$	$3.54\cdot10^{4}$
$\sum_{i\in I}\sum_{m\in M} D^{\mathrm{L1,L2}}_{i,m}\cdot f^{\mathrm{road,L1,L2}}_{i,m}\cdot q^{m,\mathrm{L1,L2}}_{i,m,\mathrm{MSW}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$3.67\cdot10^{5}$	$3.67\cdot10^{5}$	$2.95\cdot10^{5}$	0	0
$\sum_{i\in I}\sum_{m\in M} D^{\mathrm{L1,L2}}_{i,m}\cdot f^{\mathrm{road,L1,L2}}_{i,m}\cdot q^{m,\mathrm{L1,L2}}_{i,m,\mathrm{corn\ stover}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$9.19\cdot10^{5}$	$6.67\cdot10^{5}$	$4.57\cdot10^{5}$	$3.00\cdot10^{5}$	$1.33\cdot10^{5}$
$\sum_{i\in I}\sum_{m\in M} D^{\mathrm{L1,L2}}_{i,m}\cdot f^{\mathrm{road,L1,L2}}_{i,m}\cdot q^{m,\mathrm{L1,L2}}_{i,m,\mathrm{manure}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.99\cdot10^{5}$	0	0	$1.99\cdot10^{5}$	$1.82\cdot10^{5}$
$\sum_{i\in I}\sum_{m\in M} D^{\mathrm{L1,L2}}_{i,m}\cdot f^{\mathrm{road,L1,L2}}_{i,m}\cdot q^{m,\mathrm{L1,L2}}_{i,m,\mathrm{timber}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$2.17\cdot10^{5}$	0	0	$6.12\cdot10^{4}$	0
$\sum_{m\in M}\sum_{n\in N} D^{\mathrm{L2,L3}}_{m,n}\cdot f^{\mathrm{road,L2,L3}}_{m,n}\cdot q^{m,\mathrm{L2,L3}}_{m,n,\mathrm{corn\ grain}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$2.02\cdot10^{6}$	$2.08\cdot10^{6}$	$1.54\cdot10^{6}$	$1.24\cdot10^{6}$	$1.90\cdot10^{5}$
$\sum_{m\in M}\sum_{n\in N} D^{\mathrm{L2,L3}}_{m,n}\cdot f^{\mathrm{road,L2,L3}}_{m,n}\cdot q^{m,\mathrm{L2,L3}}_{m,n,\mathrm{wood\ chips}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.04\cdot10^{4}$	$2.95\cdot10^{4}$	$6.34\cdot10^{3}$	$3.69\cdot10^{4}$	$5.30\cdot10^{3}$
$\sum_{m\in M}\sum_{n\in N} D^{\mathrm{L2,L3}}_{m,n}\cdot f^{\mathrm{road,L2,L3}}_{m,n}\cdot q^{m,\mathrm{L2,L3}}_{m,n,\mathrm{MSW}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.11\cdot10^{5}$	$1.11\cdot10^{5}$	$3.31\cdot10^{4}$	0	0
$\sum_{m\in M}\sum_{n\in N} D^{\mathrm{L2,L3}}_{m,n}\cdot f^{\mathrm{road,L2,L3}}_{m,n}\cdot q^{m,\mathrm{L2,L3}}_{m,n,\mathrm{corn\ stover}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$6.30\cdot10^{5}$	$6.73\cdot10^{5}$	$3.73\cdot10^{5}$	$3.13\cdot10^{5}$	$6.00\cdot10^{4}$
$\sum_{m\in M}\sum_{n\in N} D^{\mathrm{L2,L3}}_{m,n}\cdot f^{\mathrm{road,L2,L3}}_{m,n}\cdot q^{m,\mathrm{L2,L3}}_{m,n,\mathrm{manure}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.46\cdot10^{4}$	0	0	$1.46\cdot10^{4}$	$2.92\cdot10^{4}$
$\sum_{m\in M}\sum_{n\in N} D^{\mathrm{L2,L3}}_{m,n}\cdot f^{\mathrm{road,L2,L3}}_{m,n}\cdot q^{m,\mathrm{L2,L3}}_{m,n,\mathrm{timber}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.42\cdot10^{5}$	0	0	$1.06\cdot10^{4}$	0
$\sum_{m\in M}\sum_{j\in J} D^{\mathrm{L2,L4}}_{m,j}\cdot f^{\mathrm{road,L2,L4}}_{m,j}\cdot q^{m,\mathrm{L2,L4}}_{m,j,\mathrm{corn\ grain}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	0	$1.56\cdot10^{4}$	$1.64\cdot10^{4}$	0	0
$\sum_{n\in N}\sum_{j\in J} D^{\mathrm{L3,L4}}_{n,j}\cdot f^{\mathrm{road,L3,L4}}_{n,j}\cdot q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{heat}}$, $(\mathrm{MJ}\cdot\mathrm{km})/\mathrm{y}$	$18.2\cdot10^{9}$	$13.3\cdot10^{9}$	$8.05\cdot10^{9}$	$1.30\cdot10^{9}$	$6.66\cdot10^{8}$
$\sum_{n\in N}\sum_{j\in J} D^{\mathrm{L3,L4}}_{n,j}\cdot f^{\mathrm{road,L3,L4}}_{n,j}\cdot q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{electricity}}$, $(\mathrm{MWh}\cdot\mathrm{km})/\mathrm{y}$	$5.17\cdot10^{6}$	$3.72\cdot10^{6}$	$2.21\cdot10^{6}$	$4.51\cdot10^{5}$	$1.29\cdot10^{5}$
$\sum_{n\in N}\sum_{j\in J} D^{\mathrm{L3,L4}}_{n,j}\cdot f^{\mathrm{road,L3,L4}}_{n,j}\cdot q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{ethanol}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.93\cdot10^{6}$	$1.92\cdot10^{6}$	$1.40\cdot10^{6}$	$8.53\cdot10^{5}$	$4.01\cdot10^{5}$
$\sum_{n\in N}\sum_{j\in J} D^{\mathrm{L3,L4}}_{n,j}\cdot f^{\mathrm{road,L3,L4}}_{n,j}\cdot q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{board}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$2.47\cdot10^{4}$	0	0	$7.43\cdot10^{3}$	0
$\sum_{n\in N}\sum_{j\in J} D^{\mathrm{L3,L4}}_{n,j}\cdot f^{\mathrm{road,L3,L4}}_{n,j}\cdot q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{digestate}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$9.49\cdot10^{3}$	0	0	$9.49\cdot10^{3}$	$1.03\cdot10^{4}$
$\sum_{n\in N}\sum_{j\in J} D^{\mathrm{L3,L4}}_{n,j}\cdot f^{\mathrm{road,L3,L4}}_{n,j}\cdot q^{m,\mathrm{L3,L4}}_{n,j,\mathrm{DDGS}}$, $(\mathrm{t}\cdot\mathrm{km})/\mathrm{y}$	$1.02\cdot10^{6}$	$1.05\cdot10^{5}$	$7.75\cdot10^{4}$	$5.00\cdot10^{4}$	$2.50\cdot10^{4}$

Table 6-3. Calculated environmental footprints at selected Pareto points

$F^{r}_{f,k}$ /Footprint	CF (t/(km^2·y))	WF (t/(km^2·y))	EF (GJ/(km^2·y))	WPF (t/(km^2·y))	LF (km^2/(km^2·y))
1.0	118.66	376,176.78	1,446.78	12.02	0.32
0.8	94.93	275,363.97	1,134.39	9.62	0.26
0.6	71.20	207,871.48	846.10	7.21	0.19
0.4	43.87	150,470.71	578.01	4.80	0.13
0.2	21.87	72,992.38	287.50	2.40	0.06

6.2.2 Identification of Similarities amongst Footprints

By applying the proposed measurements i) – iii) (see Section 6.1.2) for determining the similarities amongst footprints, Equations (6.2) – (6.13), at five different points, at $F^{r}_{f,k}$ = 1, 0.8, 0.6, 0.4 and 0.2, their arithmetic mean values are calculated, and are presented in Table 6-4 – Table 6-6.

Table 6-4 presents: a) the average results obtained from the first criteria, comparisons between normalised ratios regarding pairs of footprints – Equation (6.4), and b) their geometric means – Equation (6.5).

Table 6-4. a) Normalised average ratios between pairs of footprints, and b) their geometric means

		CF	WF	EF	WPF	LF
a)	CF	1.00	420.11	1.04	1.64	0.10
	WF	2.47	1.00	2.74	0.87	0.34
	EF	1.15	295.88	1.00	0.20	0.08
	WPF	1.99	1.37	2.21	1.00	0.39
	LF	3.20	1.72	3.55	1.61	1.00
b)	CF	1.00	31.55	1.09	1.66	0.56
	WF	31.55	1.00	28.48	1.09	0.76
	EF	1.09	28.48	1.00	0.67	0.53
	WPF	1.66	1.09	0.67	1.00	0.79
	LF	0.56	0.76	0.53	0.79	1.00

The ratio between footprints *f* and *ff* is equal to 1 for perfect similarity. In Table 6-4a it can be seen that when the values for normalised ratios between footprints are not close to 1, $R^{\mathrm{m}}_{f,ff}$ could differ significantly from $R^{\mathrm{m}}_{ff,f}$, e.g. $R^{\mathrm{m}}_{\mathrm{CF,WF}}$ = 420.11, whilst $R^{\mathrm{m}}_{\mathrm{WF,CF}}$ = 2.47. The selection into subsets could be achieved either from normalised average ratios (Table 6-4a) or from their geometric means (Table 6-4b). It can be seen from both Tables that two or three groups could be selected. Two groups are chosen with a higher tolerances for deviations from 1 (e.g.

± 0.25 for geometric means in Table 6-4b), the first group includes CF and EF (highlighted by the light green colour), and the second group WF, WPF, and LF (highlighted by both the medium and darker blue colours). However, with a smaller tolerances in deviations three groups are chosen, the first group includes CF and EF, the second group WF, WPF (highlighted by the darker blue colour), and the third group LF only.

Table 6-5 presents: a) the average results obtained from the second criteria, overlapping pairs of footprints in process variables (Equation (6.8)), and b) their geometric means (Equation (6.9)).

Table 6-5. a) Average overlaps of pairs of footprints in process variables, and b) their geometric means

		CF	WF	EF	WPF	LF
a)	CF	1.00	1.00	0.95	0.55	0.31
	WF	1.00	1.00	1.00	0.93	0.58
	EF	1.00	1.00	1.00	0.45	0.28
	WPF	1.00	1.00	1.00	1.00	0.62
	LF	1.00	1.00	1.00	1.00	1.00
b)	CF	1.00	1.00	0.97	0.74	0.56
	WF	1.00	1.00	1.00	0.97	0.76
	EF	0.97	1.00	1.00	0.67	0.53
	WPF	0.74	0.97	0.67	1.00	0.79
	LF	0.56	0.76	0.53	0.79	1.00

If the overlaps of pairs of footprints *f* and *ff* in the process variables are equal to 1, then footprint *f* is defined by the same process variables as footprint *ff*. Again, overlap values $O^{m}_{f,ff}$ could differ significantly from $O^{m}_{ff,f}$, e.g. $O^{m}_{\mathrm{CF,LF}} = 0.31$, whilst $O^{m}_{\mathrm{LF,CF}} = 1.00$. It can be seen from both Tables (Table 6-5a and Table 6-5b) that in the case of smaller tolerances and three subsets, the overlap values for the similar footprints are equal or very close to 1.00. In the case of larger tolerances and two subsets, the overlap values for other similar footprints and LF in the last subset are quite large (Table 6-5a), and in within ± 0.25 range in the case of geometric mean values (Table 6-5b).

It can be seen from Table 6-5b that two groups could be selected in two possible ways: i) the first group could contain CF and EF, and the second group WF, WPF, and LF, and ii) the first group could contain CF, WF, and EF, and the second group contain WPF and LF. In the first, representative footprints could not be chosen in the first group, since in this group there are only two footprints, which have the same overlap coefficients. However, from the second group WPF or WF could be chosen as representative. In the second, WF is selected as a representative footprint in the first group, since all coefficients equal 1. From the second group, the representative footprint could not be chosen since in this group there are only two footprints that have the same overlap coefficients.

Table 6-6 presents a) the average results obtained from the third criteria, average absolute normalised deviations between pairs of footprints (Equation (6.12)), and b) their arithmetic means (Equation (6.13)).

When checking absolute normalised deviation, Table 6-6a and Table 6-6b have to be considered. The smaller values indicate good agreement between pairs of footprints.

Table 6-6. a) Average absolute normalised deviations between pairs of footprints, and b) their arithmetic means

		CF	WF	EF	WPF	LF
a)	CF	0	13.99	0.01	0.79	0
	WF	0.05	0	0.07	0.03	0
	EF	0.01	9.85	0	0.12	0
	WPF	0.04	0.01	0.05	0	0
	LF	0.08	0.02	0.10	0.30	0
b)	CF	0	7.02	0.01	0.42	0.04
	WF	7.02	0	4.96	0.02	0.01
	EF	0.01	4.96	0	0.09	0.05
	WPF	0.42	0.02	0.09	0	0.15
	LF	0.04	0.01	0.05	0.15	0

Note that the deviations of footprints in pairs with LF are 0, since LF has defined just one variable, the LF of corn grain. As can be seen from Table 6-6, the deviations for similar footprints in the subsets are negligible when the smaller tolerances and three subsets are selected. When the larger tolerances are considered and two subsets selected, the values for the absolute normalised deviations and their arithmetic means, are again close to 0, except for WPF/LF ($AD^{\mathrm{m}}_{\mathrm{WPF,LF}} = 0.15$ in Table 6-6b), which is still close to 0.

From Table 6-4 – Table 6-6, it could be concluded that with a smaller tolerance three subsets of footprints could be selected (first group: CF and EF, second group: WF, WPF and third group: LF), and with larger tolerances only two subsets of footprints could be chosen (first group: CF and EF, second group: WF, WPF and LF). In the first case three representative footprints, and in the second case two representative footprints have to be selected, one from each subset.

First the two subsets are considered. The selections of representative footprints could be carried out either by considering quantitative criteria based on normalised ratios and overlapping values or qualitative criteria. When an overlap value is considered, smaller values mean that the similarities of the process variables between the first and the second footprints are smaller, whilst the similarities between the second and first are higher. This implies that the first footprints are defined with a larger number of variables to which the variables of the second footprints are just a subset. A footprint with a smaller overlap value and a larger number of variables is more suitable for selection as a representative footprint. In the first subset of similar footprints, CF is selected as the representative footprint as $O^{\mathrm{m}}_{\mathrm{CF,EF}} = 0.95$ whilst $O^{\mathrm{m}}_{\mathrm{EF,CF}} = 1.00$ (Table 6-5a). Similarly, in the second subsets WF is selected as $O^{\mathrm{m}}_{\mathrm{WF,WPF}} = 0.93$ and even $O^{\mathrm{m}}_{\mathrm{WF,LF}} = 0.58$, whilst both $O^{\mathrm{m}}_{\mathrm{WPF,WF}}$ and $O^{\mathrm{m}}_{\mathrm{LF,WF}}$ are 1.00 (Table 6-5a). Note also that the normalised average ratios between representative footprints, and other footprints within the same footprint subsets, should differ at least from 1 (Table 6-4a). The same conclusion could be obtained by considering qualitative judgement. As CF in the biomass supply chains is probably the most important footprint, WF is currently more important (Galli et al., 2012) than WPF, and LF is less important, and so for these qualitative reasons CF and WF could be selected as representative footprints.

It can be concluded that with a larger tolerance and two subsets of similar footprints CF could be selected as a representative footprint in the first subset (CF and EF), and WF in the second subset (WP, WPF and LF). In the case of a smaller tolerance LF could also be selected as a representative footprint for the third subset (LF only).

6.2.3 Multi-Objective Optimisation

In this study, MOO is only performed for two representative footprints, CF and WF, because it is more transparent, and the solutions could be better graphically represented. A 3-D problem is thus obtained; where the profit is the main criterion, and the representative footprints are constrained by ε. As a step-size $\Delta\varepsilon$ of 1 % is selected, the number of optimisation runs for the two footprints, and also the number of points within the plots is equal to 10,000.

Two scenarios of MOO are performed: (i) profit vs. representative footprints where all the remaining footprints are relaxed (optimistic scenario), and (ii) profit vs. representative footprints where the remaining footprints are constrained as their corresponding representative footprints (pessimistic scenario); EF is constrained as CF, and WPF and LF as WF. In addition, the footprints are restricted to being equal to or lower than their corresponding footprints when relaxed. The means of errors and standard deviations for optimistic (μ_o^{R} and σ_o^{R}) and pessimistic scenario (μ_o^{C} and σ_o^{C}) for each objective o are calculated from Equations (6.19) – (6.22) and shown in 3-D plots.

6.2.3.1 Optimistic scenario

Figure 6-2 shows the 3-D projection of profit vs. the two representative footprints and Figure 6-3a-c shows 3-D projections of the remaining footprints as read from the MOO solutions; 3-D projection of EF from the first subset vs. the representative footprints is represented in Figure 6-3a, and the 3-D projections of WPF and LF from the second subset are given in Figure 6-3b and Figure 6-3c.

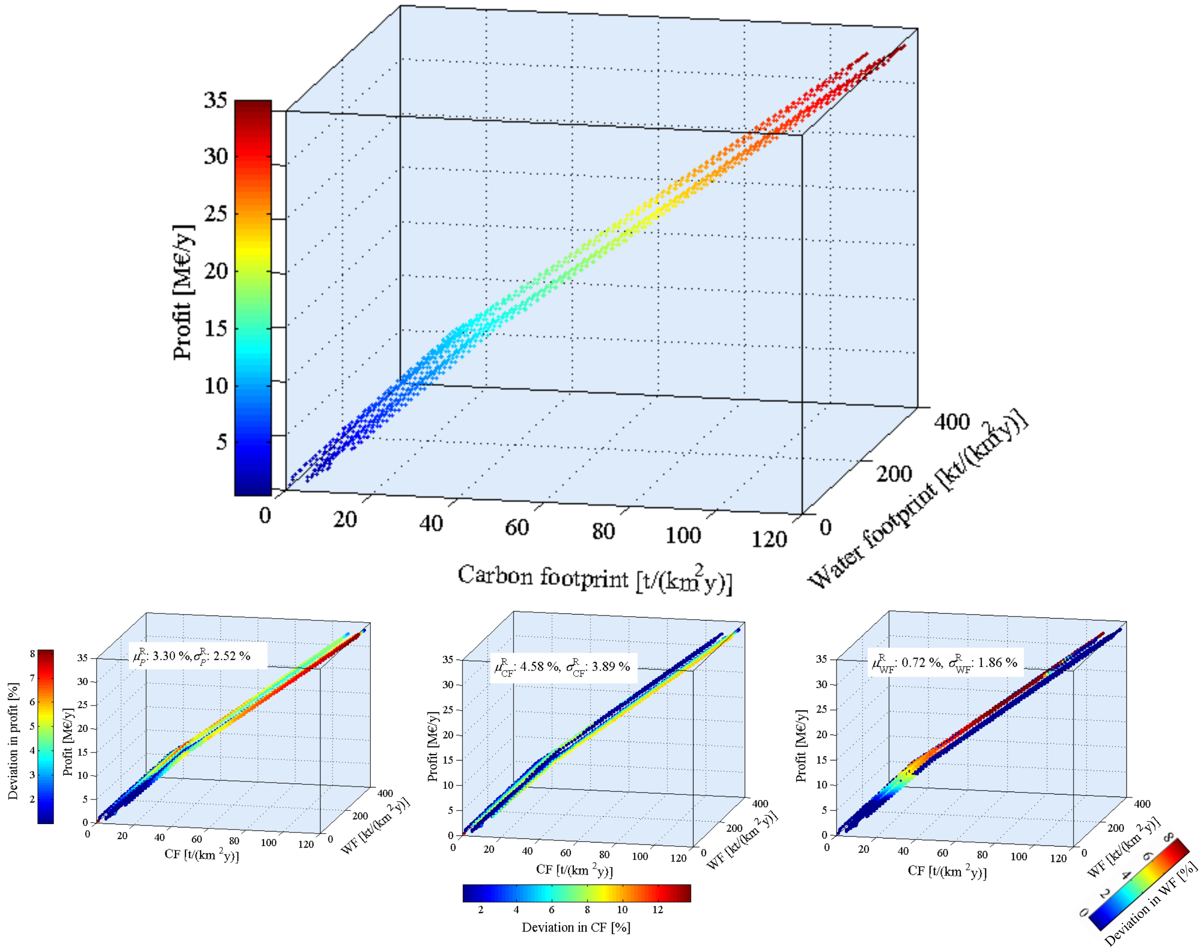
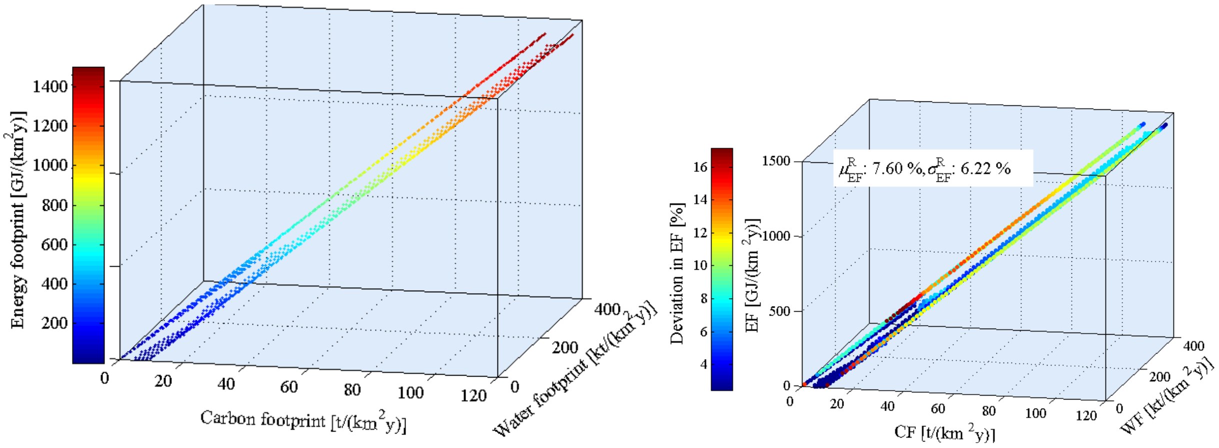


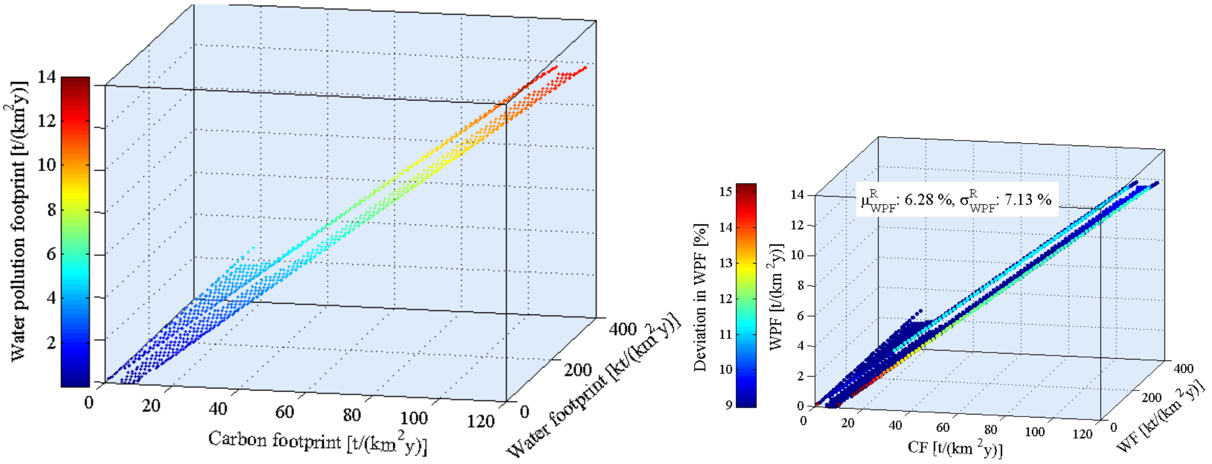
Figure 6-2. Profit vs. representative footprints within the optimistic scenario (Čuček et al., 2013a)

Removing outliers (Kreyszig, 2006) from the set of non-zero deviations, the deviations of the MOO approach are shown in smaller Figures as another D presented by colour scaling. These deviations present a measurement for the range of possible solutions between optimistic and pessimistic scenarios. Figure 6-2 presents deviation as a % of profit (on the left), in CF (in the middle) and WF (on the right), whilst Figure 6-3a, b, c presents the deviations in EF, WPF, and LF. As can be seen, the smallest deviations are associated with WP ($\mu_{\mathrm{WF}}^{\mathrm{R}}$ = 0.72 %), the medium ones with profit (μ_P^{R} = 3.30 %) and CF ($\mu_{\mathrm{CF}}^{\mathrm{R}}$ = 4.58 %), and the largest with WPF ($\mu_{\mathrm{WPF}}^{\mathrm{R}}$ = 6.28 %), LF ($\mu_{\mathrm{LF}}^{\mathrm{R}}$ = 6.57 %) and EF ($\mu_{\mathrm{EF}}^{\mathrm{R}}$ = 7.60 %).

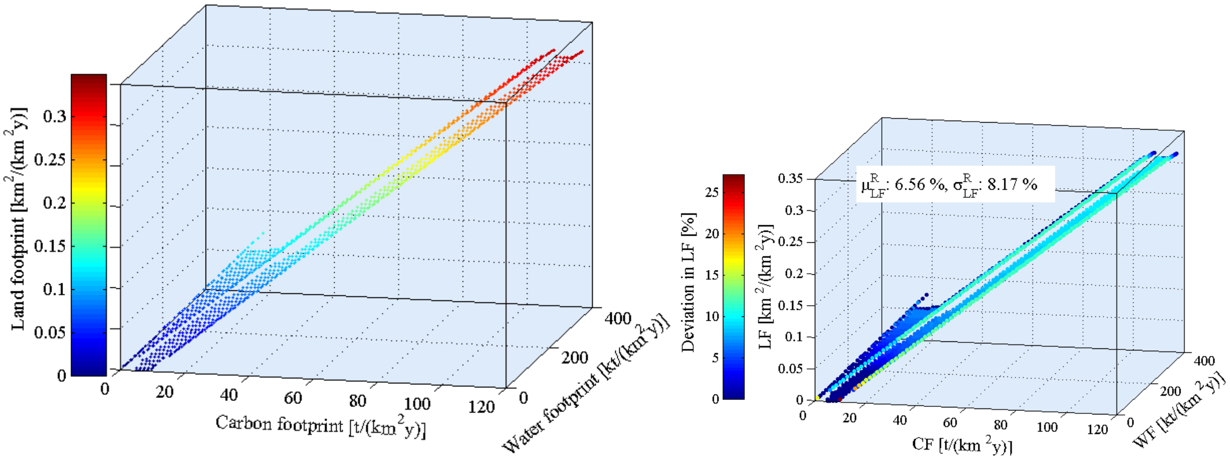
The whole range of feasible Pareto solution space and the deviation of optimistic vs. pessimistic solution for the representative footprints can be seen from Figure 6-2 and Figure 6-3. The best compromise profit-footprints solution could be selected. As the remaining footprints are not constrained, the solution space shows somewhat optimistic values for both the profit and the footprints.



a) EF from the first subset vs. CF and WF within the optimistic scenario



b) WPF from the second subset vs. WF and CF within the optimistic scenario



c) LF from the second subset vs. WF and CF within the optimistic scenario

Figure 6-3. 3-D projections of the remaining footprint vs. WF and CF in the optimistic scenario: a) for EF from the first subset, b) for WPF and c) LF from the second subset (Čuček et al., 2013a)

6.2.3.2 Pessimistic scenario

Figure 6-4 also shows the results for the profit vs. the representative footprints obtained by MOO, where the remaining footprints are as constrained as their corresponding representative footprints; EF is constrained as CF, and WPF and WF are constrained as WF, and additionally these footprints have to be either equal or lower than those obtained by the optimistic scenario. 3-D projections of the remaining footprints are plotted in Figure 6-5a for EF from the first subset, and in Figure 6-5b, c for WPF and LF from second subset.

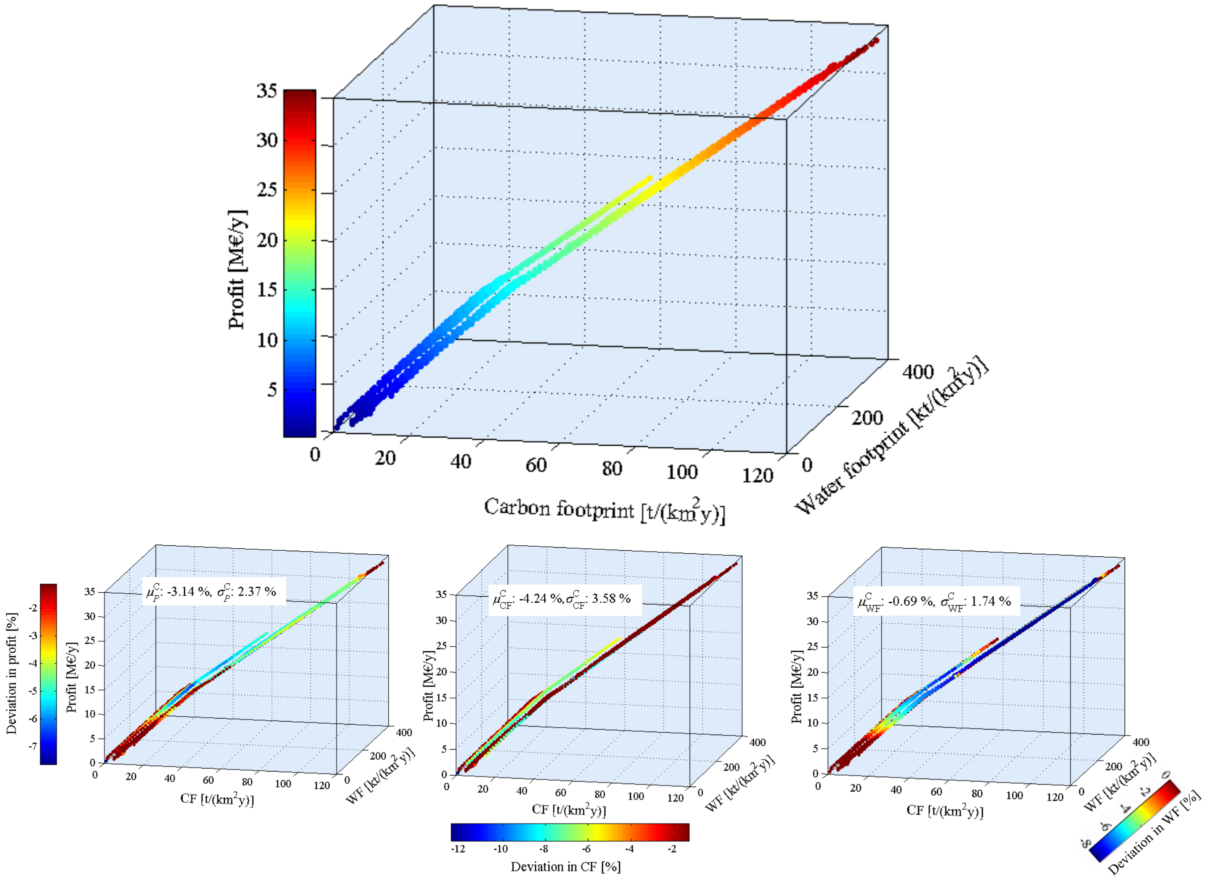
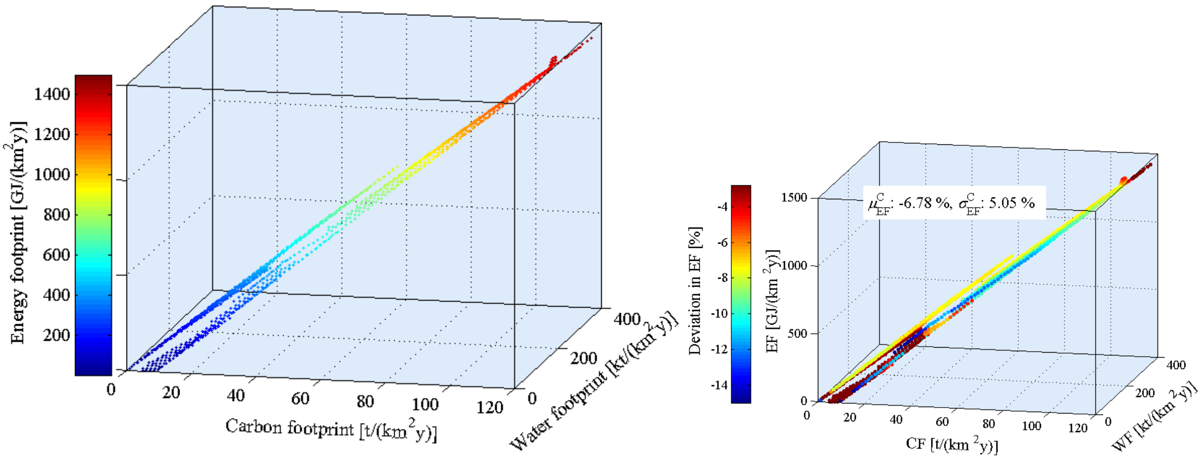
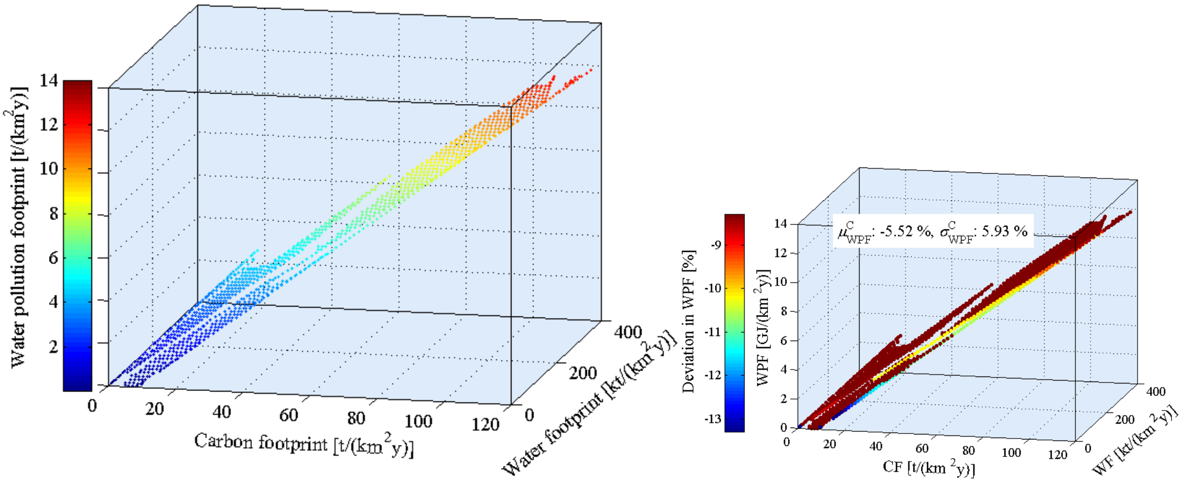


Figure 6-4. Profit vs. representative footprints within the pessimistic scenario (Čuček et al., 2013a)

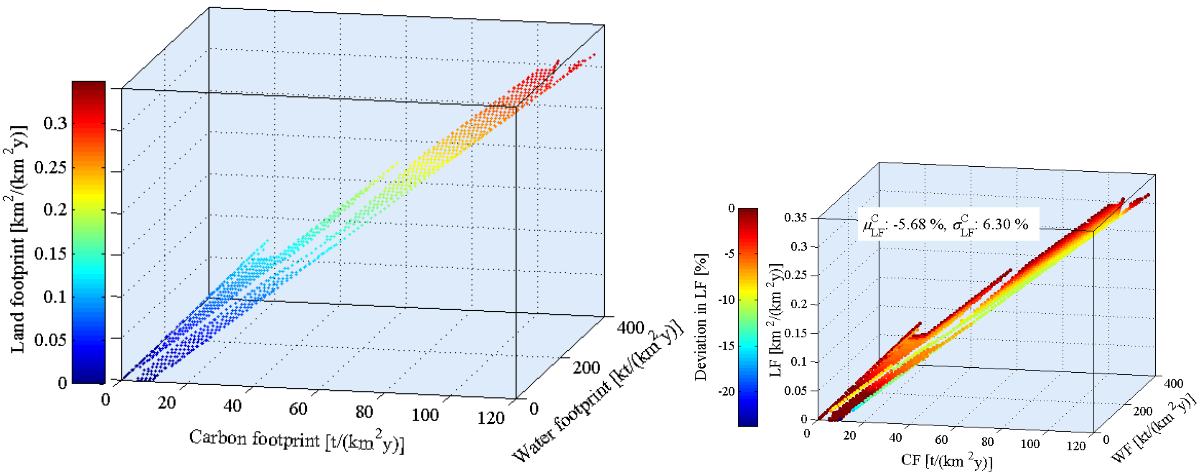
The smaller Figure 6-4 and Figure 6-5 again show the errors of the MOO approach, and present the range of possible solutions between pessimistic and optimistic scenarios. The Figures show the percentage deviations as compared with the optimistic scenario, as another dimension presented by colour scaling; Figure 6-4 presents deviation as a % for profit (on the left), CF (in the middle), and WF (on the right), whilst Figure 6-5a presents the deviation in EF, Figure 6-5b deviation in WPF, and Figure 6-5c deviation in LF.



a) EF from the first subset vs. CF and WF within the pessimistic scenario



b) WPF from the second subset vs. WF and CF within the pessimistic scenario



c) LF from the second subset vs. WF and CF within the pessimistic scenario

Figure 6-5. 3-D projections of the remaining footprints vs. WF and CF in the pessimistic scenario: a) for EF from the first subset, b) for WPF and c) LF from the second subset (Čuček et al., 2013a)

As can again be seen, the smallest deviations are associated with WF ($\mu_{\mathrm{WF}}^{\mathrm{C}}$ = -0.69 %), the medium ones with profit (μ_{P}^{C} = -3.14 %) and CF ($\mu_{\mathrm{CF}}^{\mathrm{C}}$ = -4.24 %), and the largest with WPF ($\mu_{\mathrm{WPF}}^{\mathrm{C}}$ = -5.52 %), LF ($\mu_{\mathrm{LF}}^{\mathrm{C}}$ = -5.68 %) and EF ($\mu_{\mathrm{EF}}^{\mathrm{C}}$ = -6.78 %). The negative values indicate that objectives obtained from the pessimistic solutions are smaller than those from the optimistic solutions.

As all the remaining footprints are now constrained the same way as their representative footprints, and restricted to being equal or lower than those obtained at an optimistic scenario, the Pareto solution space is more constrained and shows a tendency towards lower values for profit. It can be seen from Figure 6-4 and Figure 6-5 that the range of feasible solution space for footprints at given profits has been enlarged when compared to the optimistic scenario.

As to which option to select, optimistic, compromise or pessimistic, depends on the decision-makers. It is suggested in favour of the optimistic scenario. Rather good environmental solutions could still be obtained even if the remaining footprints are relaxed, giving rise to somewhat overestimated profit solutions. The remaining footprints actually have similar behaviour as their corresponding representative footprints anyway, and therefore their solutions could not be far from the optimistic solution, and they also have higher profits.

In order to summarise the presented novel ROM method, by which the number of direct environmental footprints in MOO is reduced to a minimum number of representative footprints, the procedure is briefly outlined in the following:

i) Definition of the MOO model and identification of matrix coefficients.
ii) Generation of appropriate points for determining similarities amongst footprints performing 2-D MOO by maximising profit vs. equally-constrained all footprints.
iii) Identifications of similarities amongst footprints using the criteria as in Equations (6.2) – (6.13).
iv) Groupings of the representative and remaining footprints into subsets containing footprints with similar behaviour. Applying normalised average ratios between footprints as the main grouping criteria.
v) Selection of representative footprints. Identification is performed by quantitative (normalised overlaps in process variables and normalised average ratios) and qualitative judgement.
vi) Performing MOO with representative footprints, by relaxing the remaining footprints.
vii) Representation of multi-D projections of profit vs. representative footprints, and remaining footprints vs. representative footprints.

7 CONCLUSIONS AND FUTURE WORKS

This PhD thesis presented a systematic approach for the synthesis of sustainable bioprocesses, integrated bioprocesses and supply chain networks. The MP approach was applied for the synthesis that enables the obtaining of optimal solutions, or several sets of Pareto optimal solutions from the economic and environmental points of view.

This dissertation was divided into several Chapters, amongst them being the four main Chapters, that contained the majority of the research work within the framework of this thesis, i) synthesis of integrated bioprocesses, ii) synthesis of regional biomass energy networks, iii) methods for evaluating the sustainable development within MOO when considering biomass energy production, and a final main Chapter that dealt with the reduction of dimensionality of the criteria within MOO.

The first part of the work dealt with the simultaneous integration of technologies, raw materials, and energy towards the sustainable production of ethanol from the entire corn plant. The process was modelled and solved using the process synthesiser MIPSYN, which proved to be a powerful tool for analysing a large number of trade-offs implemented within the problem formulation. It was found that the most economical process was based on the thermo-chemical route, whilst the most economically-integrated process consisted of the thermo-chemical route and the dry-grind process, due to the large impact of the HI that can be achieved. Whilst in the short-term, the production of ethanol from corn grain and stover can co-exist, the lignocellulosic material would eventually displace the use of grain to its lower cost. There is a need for a more detailed analysis and pilot plants to verify the results of the proposed integrated process. However, these results provide a potentially promising bridge between the first and second generations of bioethanol.

The second part of the work presented a developed general optimisation model for the bioenergy production supply chain at a regional level. Firstly, a simplified model was developed, which was further extended into a more comprehensive heat-integrated multi-period model. Using the developed models, it was possible to optimise the production chains within each regional area, depending on the availability and suitability of the biomass resources. The models offered a powerful tool for synthesising biomass energy supply chain networks. From the more comprehensive model and the illustrative example of the biorefinery's supply chains incorporating first, second, and third generations of biofuels it could be concluded that biomass and waste, especially switchgrass and algae, are promising raw materials for producing biofuels. It has been demonstrated that it is feasible to economically produce second and third generations of biofuels with significant profit. Even higher profits (for around 40 %) could be obtained by the variable usage of agricultural areas because of lower storage costs and by avoiding the limitations of capacities within the various technologies. It was also demonstrated that producing biofuels was more economically sounder as producing food, and that by using 20 % of the land area the demand for food and transportation fuels could be satisfied when applying the world and EU demand patterns. However, when applying the US average demand pattern for transportation fuels, the area required to satisfy the demand for food and transportation fuels increased to 60 %.

The third main part of the work, the development of different assessment methods for measuring sustainable development, is divided into three subchapters: footprints, sustainability indexes and eco-profit, total profit and other combined criteria. The first subchapter presented a MOO of the regional biomass and bioenergy supply chains in order to maximise the economic performances of the supply chains by simultaneously minimising different footprints. Direct, indirect and total footprints were studied in the MOO approach. It was seen from the optimisation of the total footprints that CF and EF were reduced, whilst WF, WPF and LF were increased compared to the conventional mainly fossil energy. Biomass energy compared to conventional energy requires much more water, transport, chemicals, causes the pollution of water, and also requires large land areas. CF and EF, on the one hand, and WF, WPF and LF, on the other hand, showed similar behaviour. It was clear that product substitution could have a significant effect on the footprints and therefore should be considered. The results indicated that considering total effects enables the obtaining of more realistic solutions than in those cases when considering only direct effects.

The second subchapter presented a MOO approach based on RDSI and RTSI, performed on the illustrative example of an integrated biogas process with or without a rendering plant. The results indicated that biogas production is an unsustainable alternative when considering only direct effects (burdening) on the environment; whilst when also considering indirect effects (unburdening), the analysis revealed that biogas production is a sustainable alternative that benefits the environment. The indirect sustainability indicators were prevalent, and the total sustainability indicators were negative, except for the LF. By lowering the RDSI, the production of biogas products lowered, and approached zero, as also did the profit. The solutions that comprise only direct effects, did not show the right pathway towards improvements within the systems. When only the RDSI was used, biogas production from animal and other organic waste seemed to be unsustainable. It was demonstrated that indirect effects caused by utilising harmful waste and by products’ substitution should also be considered, besides the direct effects. The selection of alternatives that unburden the environment the most, should have higher priority than the rejection of those with only smaller burdening impacts. It was seen that total sustainability indicators were very negative (positive for the environment), as well as the RTSI at the optimal solution (RTSI ≈ -3.740 for a maximal profit of 3.668 M€/y). By considering RTSI it was seen that, instead of non-inferior trade-off Pareto solutions, as in the case of RDSI, a set of non-trade-off solutions was obtained where, at the highest economic profits the best environmental solutions were also identified.

The third subchapter presented a novel LCA-based MP approach, based on the concept of eco-profit and total profit demonstrated by the example of an integrated biogas process from animal and other organic wastes. Also, all the results from SOO and MOO showed that biogas production is a sustainable alternative, which provides benefits for the environment and important eco-profit and total profit. The results obtained by the maximisation of the total profit indicated the appropriate trade-off between economic profit and eco-profit. Maximised total profit, eco-profit, and economic profits were significant (6.508, 2.667, and 3.668 M€/y), and therefore it can be concluded that the production of biogas is an economically and environmentally-attractive solution that unburdens the environment.

The fourth and the last main part of the work introduced a methodology (principle and procedure) based on a novel ROM for the identification of similarities amongst different objectives (footprints) within MOO. The presented dimensionality reduction method is applicable in those cases where the model is known. The number of footprints was reduced through similarities amongst those footprints that show similar behaviour. Two scenarios in terms of the remaining footprints were performed and presented, an optimistic scenario where the remaining footprints were relaxed, and a pessimistic scenario where the remaining footprints were constrained as their representative footprints. Following the presented procedure, the dimensionality of the criteria set can be significantly reduced to a minimum number of representative footprints. The presented methodology offers several advantages, such as results are presented in multi-D projections for footprints directly as obtained from optimisation solutions. Any error, usually associated with correlation calculations, is thus circumvented; however, there was deviation in the results from optimistic and pessimistic scenarios. Since this method deals with footprints directly, the subjective weighting of footprints as for the environmental index, is thus avoided. This method is simple and can be easily implemented. The methodology was successfully applied to an illustrative example of biomass energy supply chains where the dimensionality of footprints was reduced from five to two. The illustrative example indicated that using the novel approach makes MOO more practical for real-life problems and decision making.

In the future appropriate model reduction techniques and efficient decomposition approaches will be needed within the multi-period optimisation model for bioenergy production supply chains in order to apply the synthesis model over wider areas and entire regions, possibly even countries. In order to account for regional characteristics, the presented model and case study will need to be applied over wider area and specific regions, such as e.g., within EU.

The developed generic synthesis model for efficient bioenergy network optimisation, presented in Section 4.2.1, should be further upgraded to account for different modes of transport and distribution, such as road, rail and ship transport of biomass resources and products, and pipeline delivery of liquid fuels and hydrogen. Furthermore, direct, indirect, and total environmental impacts will need to be evaluated within the multi-period optimisation models in order to obtain economically-efficient and environmentally-benign solutions. Finally, this model should be extended to account for different uncertainties relating to fluctuations in supplies and demands, prices and other data. A multi-objective multi-period optimisation model under uncertainty will therefore evolved into an efficient supporting tool for decision-making within regional energy planning and management.

Eco-profit, net profit and total profit concepts can be extended to the concept of eco-, net and total NPV. NPV is an economic measurement that properly takes into account the complete economics of the project throughout the project’s life cycle. The eco-NPV is an analogy of the economic NPV, where income within the NPV’s yearly cash-flow is represented by unburdening (eco-benefit) and the outcome by a burdening (eco-cost) on the environment. Eco- and total NPVs also enables the inclusion of environmental and economic dimensions of SD within one measurement, expressed as a monetary value. The preferred solutions are those with maximal total NPV.

The ROM methodology should be further upgraded to those cases where the model is unknown. The presented approach was namely based on the matrix coefficients from the model, as well as the calculated process variables at their selected Pareto optimal values. By upgrading this presented methodology to unknown models, the methodology would become universally applicable. Furthermore, the similarities amongst footprints should also be investigated regarding several other footprints, such as nitrogen, phosphorus, and biodiversity footprints. It should be noted that only direct environmental footprints were presented during this dissertation when reducing the dimensionality of the MOO problem. In order to achieve more realistic solutions, the indirect (unburdening) effects should be included in addition to the direct, thus considering the total effects (burdening and unburdening).

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BIOGRAPHY

Europass Curriculum Vitae

Personal information

First name(s) / Surname(s)	**Lidija ČUČEK**
E-mail	lidija.cucek@um.si
Citizenship	Slovenian

Work experiences

Dates	**October 2008 –**
Occupation or position held	Junior researcher and assistant
Main activities and responsibilities	Research on the topic of Synthesis of sustainable bioprocesses using computer-aided process engineering Assistant for courses Process Integration, Process Development, Process Dynamics, Computer Aided Process Design and Process Synthesis
Name and address of employer	University of Maribor, Faculty of Chemistry and Chemical Engineering Smetanova 17, SI-2000 Maribor, Slovenia
Dates	**2007**
	Work experience on the Faculty of Chemistry and Chemical Engineering, University of Maribor
Main activities and responsibilities	Modelling of process units for optimisation of ethanol plants. Simulation and optimisation of ethanol production using GAMS and MIPSYN.
Name and address of employer	University of Maribor, Faculty of Chemistry and Chemical Engineering Smetanova 17, SI-2000 Maribor, Slovenia
Dates	**2006**
	Work experience in histological laboratory in the Department of pathological morphology, General Hospital Maribor
Main activities and responsibilities	Duties in the laboratory, samples preparation, analysis of the samples by different methods. Determination of the presence of cancer cells.

Name and address of employer	General Hospital Maribor, Ljubljanska ulica 5, SI-2000 Maribor, Slovenia
Dates	**2005 – 2007**
	Working in the production
Main activities and responsibilities	Working in the production in Department of a service activity, plastics, cosmetics and hair colours. In most cases working at an assembly line.
Name and address of employer	Henkel Slovenija d.o.o. Industrijska ulica 23, SI-2506 Maribor, Slovenia
Dates	**2004 – 2007**
	Working through the student service
Main activities and responsibilities	Marketing and services in various professions as a part of a student holiday and extra time work (including work in production, work in call centre, instruction of chemistry and mathematics, etc.)

Education and training

Dates	**2011 –**
Title of qualification awarded	PhD
Principal subjects/occupational skills covered	PhD topic: Life Cycle Assessment and Supply Chain Optimisation with the Targeting the Emissions (including CO_2) and Effluent Reduction. The Extension of Footprint and Sustainability Indexes Methodology
Name and type of organisation providing education and training	University of Pannonia, Faculty of Information Technology, Egyetem utca 10, HU-8200 Veszprém, Hungary
Dates	**2008 –**
Title of qualification awarded	PhD
Principal subjects/occupational skills covered	PhD topic: Synthesis of sustainable bioprocesses using computer-aided process engineering
Name and type of organisation providing education and training	University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova 17, SI-2000 Maribor, Slovenia
Dates	**2003 – 2008**
Title of qualification awarded	University Degree in Chemical Engineering, equivalent to Master
Principal subjects/occupational skills covered	Title of undergraduate thesis: Optimisation of corn-based ethanol plants with process synthesizer MIPSYN

Name and type of organisation providing education and training	University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova 17, SI-2000 Maribor, Slovenia
Dates	**October 2006 – March 2007**
Name and type of organisation providing education and training	ERASMUS student exchange Friedrich – Aleksander University of Erlangen - Nürnberg, Department of Chemical and Bioengineering, Cauerstrasse 4, 91058 Erlangen, Germany
Dates	**1999 – 2003**
Name and type of organisation providing education and training	III. Grammar School of Maribor, Gosposvetska cesta 4, SI-2000 Maribor, Slovenia

Personal skills and competences

Mother tongue(s)	**Slovenian**
Other language(s)	

Self-assessment	**Understanding**		**Speaking**		**Writing**
European level (*)	Listening	Reading	Spoken interaction	Spoken production	
English	C1	C1	B2	B2	C1
German	B2	B2	B1	A2	B2

(*) Common European Framework of Reference for Languages

Computer skills and competences	Advanced knowledge of Microsoft Office (Word, Excel, PowerPoint), modelling systems for mathematical programming and optimisation GAMS and MIPSYN, software SuperPro Designer Knowledge of programming language and computing environment Matlab, Scilab, GNU Octave and Wolfram Mathematica, tool for modelling, simulating and analysing dynamic systems Simulink and Berkeley Madonna, and the software for Life Cycle Assessment GaBi Basic knowledge of graphic design applications (CorelDraw, SmartDraw), softwares Aspen Plus, Aspen Icarus, Mathcad, programming languages and computing environments Fortran, finite element analysis software environment COMSOL Multiphysics Basic knowledge and some experience with HTML and web page design with Macromedia Dreamweaver and Macromedia Fireworks and some experience with PHP code (phpBB web forum)

Driving licence	From 12.04.2005 for B category
Hobbies	Sport, travelling, dancing, swimming

Bibliography

International Journals with Impact Factor

1. Čuček L., Lam H.L., Klemeš J.J., Varbanov P. S., Kravanja Z., 2010, Synthesis of regional networks for the supply of energy and bioproducts, Clean Technologies and Environmental Policy, 12(6), 635-645 (IF = 1.753 in 2011) (32 citations on March 9, 2013) – the second most cited paper published in CTEP in last years
2. Čuček L., Martín M., Grossmann I.E., Kravanja Z., 2011, Energy, water and process technologies integration for the simultaneous production of ethanol and food from the entire corn plant, Computers and Chemical Engineering, 35(8), 1547-1557 (IF = 2.320 in 2011) (16 citations on March 9, 2013)
3. Čuček L., Varbanov P.S., Klemeš J.J., Kravanja Z., 2012, Total footprints-based multi-criteria optimisation of regional biomass energy supply chains, Energy, 44(1), 135-145 (IF = 3.487 in 2011) (11 citations on March 9, 2013)
4. Čuček L., Drobež R., Pahor B., Kravanja Z., 2012, Sustainable synthesis of biogas processes using a novel concept of eco-profit, Computers and Chemical Engineering, 42, 87-100 (IF = 2.320 in 2011) (6 citations on March 9, 2013)
5. Kravanja Z., Čuček L., 2013, Multi-objective optimisation for generating sustainable solutions considering total effects on the environment, Applied Energy, 101, 67-80 (IF = 5.106 in 2011) (5 citations on March 9, 2013)
6. Čuček L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2013, Dealing with high-dimensionality of criteria in multi-objective optimisation of biomass energy supply networks, Industrial and Engineering Chemistry Research, doi: 10.1021/ie302599c (IF = 2.237 in 2011)
7. Čuček L., Martín M., Grossmann I.E., Kravanja Z., 2013, Multi-period synthesis of optimally-integrated biomass and bioenergy supply network, Computers & Chemical Engineering (IF = 2.320 in 2011)

International Peer-Reviewed Papers

8. Čuček L., Kravanja Z., 2010, Sustainable LCA-based MINLP synthesis of bioethanol processes, Computer Aided Chemical Engineering, 28, 1889-1894 (4 citations on March 9, 2013)
9. Čuček L., Lam H.L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2010, Synthesis of networks for the production and supply of renewable energy from biomass, Chemical Engineering Transactions, 21, 1189-1194 (5 citations on March 9, 2013)
10. Čuček L., Martín M., Grossmann I.E., Kravanja Z., 2011, Energy, water and process technologies integration for the simultaneous production of ethanol and food from the entire corn plant, Computers Aided Chemical Engineering, 29, 2004-2008
11. Čuček L., Drobež R., Pahor B., Kravanja Z., 2012, Sustainable LCA-based MIP synthesis of biogas processes, Computers Aided Chemical Engineering, 29, 1999-2003 (1 citation on March 9, 2013)
12. Čuček L., Klemeš J.J., Kravanja Z., 2012, Accessing direct and indirect effects within a LCA-based multi-objective synthesis of bioproducts supply chains, Computer Aided Chemical Engineering, 31, 1065-1069
13. Čuček L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2012, Correlations among footprints within biomass energy supply chains, Computer Aided Chemical Engineering, 31, 1397-1401 (1 citation on March 9, 2013)
14. Čuček L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2012, Reducing the dimensionality of criteria in multi-objective optimisation of biomass energy supply chains, Chemical Engineering Transactions, 29, 1231-1236
15. Čuček L., Martín M., Grossmann I.E., Kravanja Z., 2013, Multi-period synthesis of a biorefinery's supply networks, Computer Aided Chemical Engineering, accepted for publication
16. Čuček L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2013, Dimensionality Reduction Approach for Multi-Objective Optimisation Extended to Total Footprints, Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA), Kuala Lumpur, Malaysia, accepted for publication

Conference Proceedings

17. Čuček L., Kravanja Z., 2010, LCA-based synthesis of a bioethanol production network, AIChE Spring Meeting and 6th Global Congress on Process Safety, 21-25 March 2010, San Antonio, Texas, US
18. Čuček L., Lam H.L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2010, Multi-objective synthesis of regional networks for the integrated production and consumption of renewable energy and food, 37th International Conference of Slovak Society of Chemical Engineering, 24-28 May 2010, Tatranské Matliare, Slovakia
19. Čuček L., Kravanja Z., 2010, Multi-technology heat integrated bioethanol production processes, 37th International Conference of Slovak Society of Chemical Engineering, 24-28 May 2010, Tatranské Matliare, Slovakia
20. Čuček L., Lam H.L., Klemeš J.J., Varbanov P.S., Kravanja Z., 2010, Multi-objective synthesis of regional networks for the integrated production and consumption of renewable energy and food, Slovenian Chemical Days, 23 and 24 of September 2010, Maribor, Slovenia
21. Čuček L., Drobež R., Pahor B., Kravanja Z., 2011, Sustainable synthesis of biogas process by the simultaneous consideration of economic and eco-profit, Slovenian Chemical Days, 14-16 September 2011, Portorož, Slovenia
22. Čuček L., Kravanja Z., 2011, Multi-objective footprints-based synthesis of integrated bioethanol production systems, AIChE Annual Meeting, Minneapolis, Minnesota, US
23. Čuček L., Martín M., Grossmann I.E., Kravanja Z., 2012, Synthesis of optimally-integrated biomass and bioenergy supply network, Slovenian Chemical Days, 12-14 September 2012, Portorož, Slovenia
24. Čuček L., Martín M., Grossmann I.E., Kravanja Z., 2012, Multi-objective optimization of a biorefinery's supply network, AIChE Annual Meeting, 28 October – 2 November 2012, Pittsburgh, Pennsylvania, US

Invited Lecture

25. Kravanja Z., Čuček L., 2011, Considering the direct and indirect environmental effects in a multi-objective synthesis of bioenergy systems, lecture presented at Carnegie Mellon University, Department of Chemical Engineering, 25 October 2011, Pittsburgh, Pennsylvania, US
26. Kravanja Z., Čuček L., 2012, CAPE for sustainable development considering the direct and indirect environmental effects in a multi-objective synthesis of sustainable systems, plenary lecture presented at CAPE FORUM, 26-28 March 2012, Veszprém, Hungary

Invited Reviewer for International Journals with Impact Factor

27. Applied Energy (Elsevier, UK)
28. Applied Thermal Engineering (Elsevier, UK)
29. Clean Technologies and Environmental Policy (Springer, US) – among outstanding reviewers for CTEP in 2012
30. Computers and Chemical Engineering (Elsevier, US)
31. Fruits (EDP Sciences, France)
32. Journal of Cleaner Production (Elsevier, US)
33. Latin American Applied Research (PLAPIQUI Planta Piloto de Ingenieria Quimica, CONICET / Universidad Nacional del Sur, Argentina)
34. Theoretical Foundations of Chemical Engineering (Springer, Russia)

UNIVERZA V MARIBORU
FAKULTETA ZA KEMIJO IN KEMIJSKO TEHNOLOGIJO

IZJAVA DOKTORSKEGA KANDIDATA

Podpisani-a **Lidija Čuček**, vpisna številka **95033018**

izjavljam,

da je doktorska disertacija z naslovom

Synthesis of sustainable bioprocesses using computer-aided process engineering

- rezultat lastnega raziskovalnega dela,
- da predložena disertacija v celoti ali v delih ni bila predložena za pridobitev kakršnekoli izobrazbe po študijskem programu druge fakultete ali univerze,
- da so rezultati korektno navedeni in
- da nisem kršil-a avtorskih pravic in intelektualne lastnine drugih.

Podpis doktorskega-e kandidata-ke:

Lidija Čuček