LCA-Based Multiobjective Synthesis of Sustainable Systems

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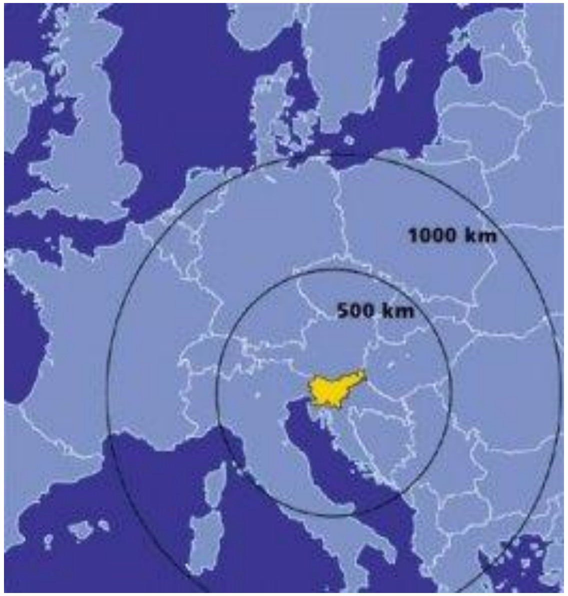

Slovenia in Pictures

Area: 20,273 km2
Population: 2.0 million
Capital city: Ljubljana
Language: Slovenian; also Italian and Hungarian in nationally mixed areas
Currency: EURO, €
Member of EU - 1 May 2004
EU Presidency for 2008

MARIBOR2012
European Capital of Culture

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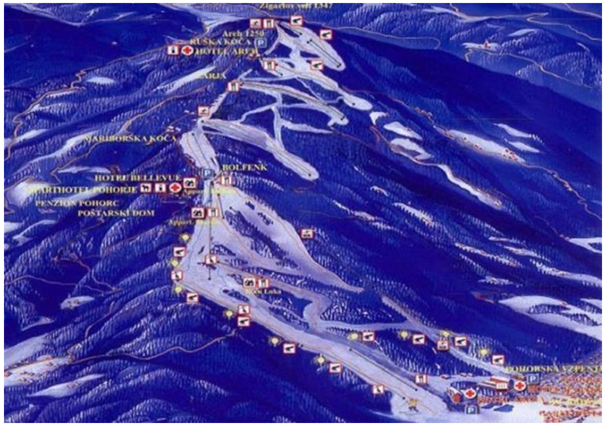


OUTLINE

- Incentives for Sustainable Development
- LCA-based Mathematical Programming for Sustainable System Synthesis
- Expanding Systems Boundaries
- Tools and Concepts Integration
- New Concept Considering Burdening and Unburdening Effects on Environment in Multiobjective Optimization:
    - Total Footprints,
    - Total Sustainability Index, and
    - Eco-Profit and Total Profit
- Synthesis Applications of Renewables Integration and Bioenergy Production
- Conclusion

1.1 Exponential Rise of Civilization

After Michio Kaku, Hyperspace, 1994

Classification of future civilizations by Nikolai Kardashev

	Scale of power:
• Type I - Controls the energy of entire planet (weather, earthquakes, mines deep into the core, harvests the oceans)	10^{15} W
• Type II – Control the power of the sun (mines it and directly consumes its energy)	10^{20} - 10^{25}W
• Type II – Controls the power of the whole galaxy (probably manipulates space-time continuum)	10^{25} - 10^{30} W

For further flourish of our civilization new inventions for mass to energy transformation ($E=m.c^2$) would be needed!

Where are We Today?
Word Energy Consumption

Type 0 Civilization - 14 TW

Quadrillion Btu=1.055 10^{18} J

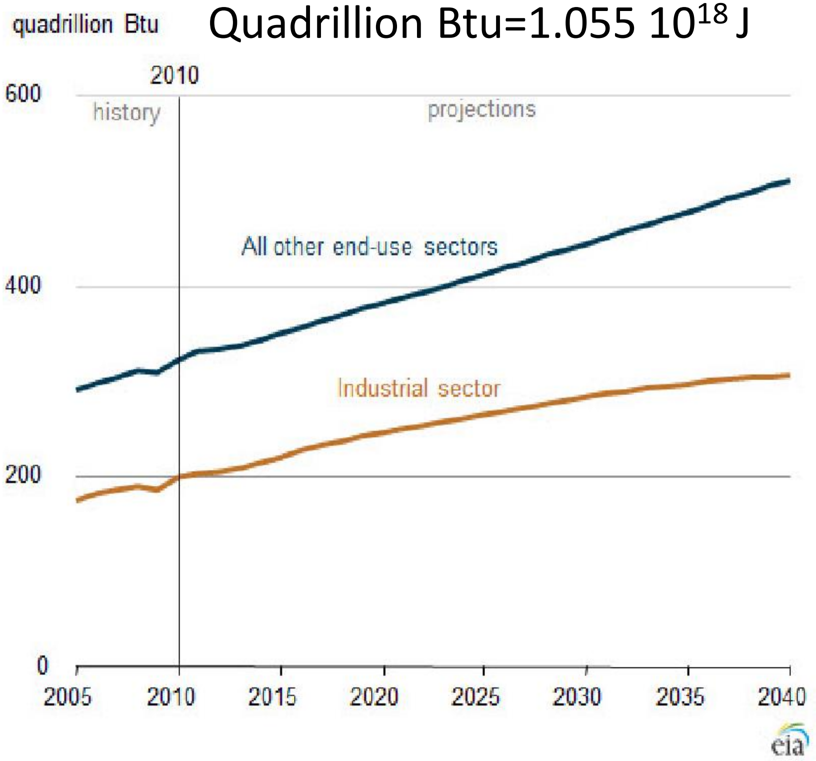


Fig. 1: World delivered end-user energy consumption

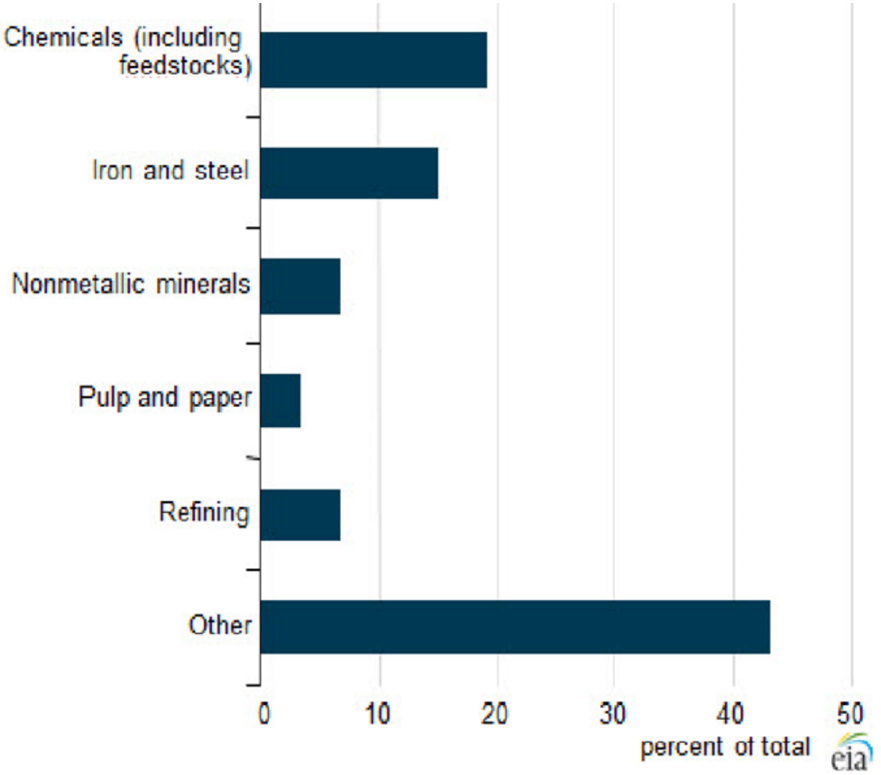


Fig. 2: Shares of world industrial sector delivered energy consumption, 2010

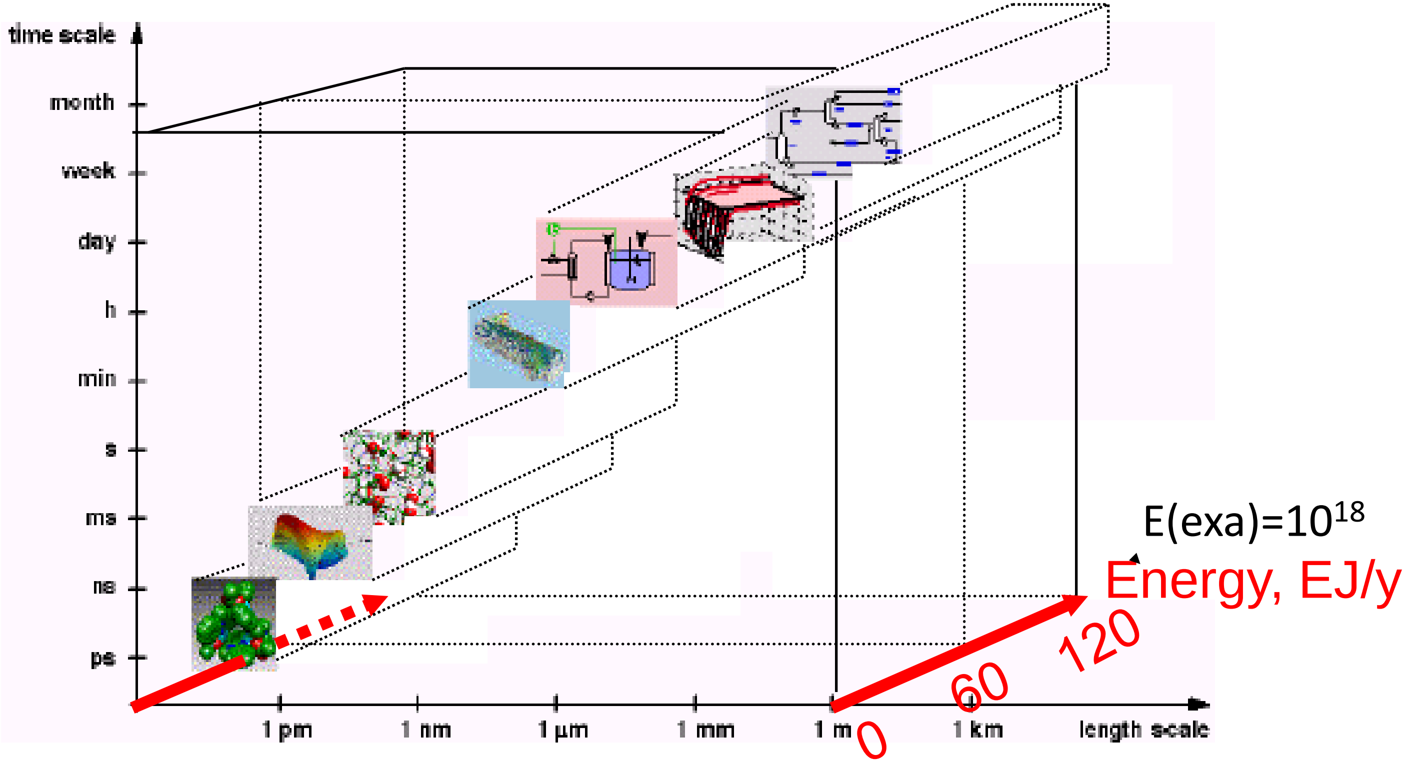
Source: International Energy Outlook 2013, U.S. Energy Andministration Angency, http://www.eia.gov/forecasts/ieo/industrial.cfm

Chemical and Process Industies Energy Consumption

- Separation processes alone represent about 15%, or even 25% of total world energy consumption!

Koros WJ. <energy.gatech.edu/questions/koros.php>; 2011

TUDelta. <delta.tudelft.nl/article/dow-awards-separation-by-freezing/24054>



After Marquardt Wolfgang, Lars Von Wedel, and Birget Bayer. AspenWorld 2000, Orlando, FL, 2000

Figure 3: Energy involved in chemical and process industries

Unsustainable Use of Energy Resources

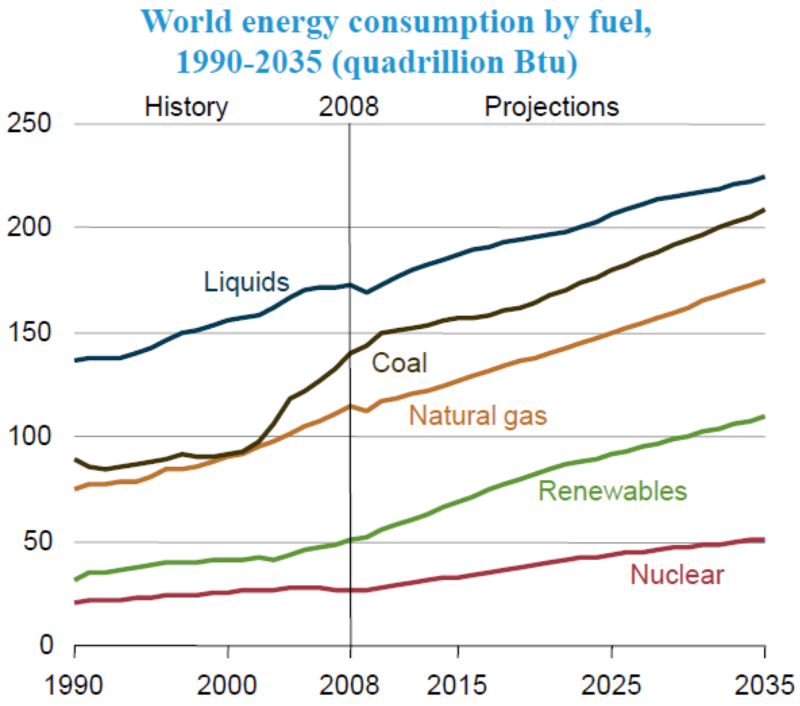


Fig. 4: World marketed energy consumption

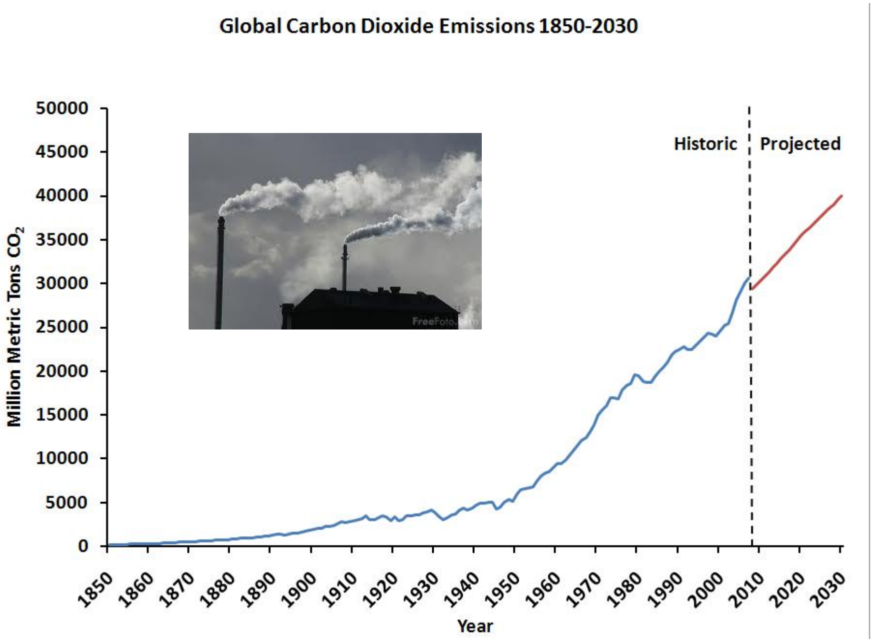


Fig. 5: Global carbon emissions from fossil fuel burning

Source: Energy Information Administration (EIA), International Energy Outlook 2011, World energy consumption by fuel 1990-2035, www.eia.doe.gov/iea/http://www.eia.gov/forecasts/ieo/highlights.cfm. Accessed 23.08.2012

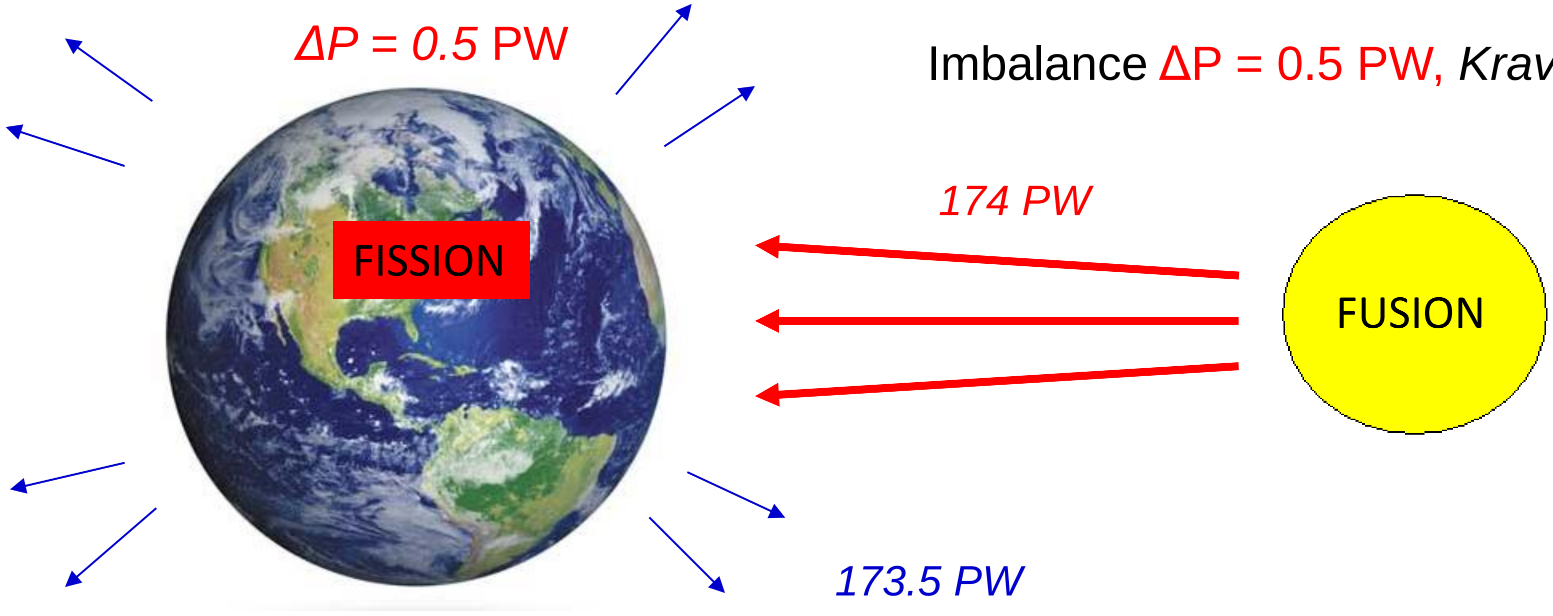
Source: Center for climate and energy solutions, Historical global CO_2 emissions, www.c2es.org/facts-figures/international-emissions/historical. Accessed 23.08.2012

1.2 Global Energy System

Climate forcing 0.85 ± 0.15 W/m², *Hansen J, 2005*

Around 1 W/m², *Meehl et al., 2011*

Imbalance ΔP = 0.5 PW, *Kravanja, 2012*



ΔP = 0.5 PW

FISSION

174 PW

FUSION

173.5 PW

Balance (PW): Accumulation = Inlet - Outlet

$$\frac{\mathrm{d}\Phi}{\mathrm{d}t} = 174 - 173.5 = +0.5\ \text{PW}$$

From Sun - (Reflected + Radiated)

Figure 6: Systems analysis when applied to the global energy system

Global Temperature Rise

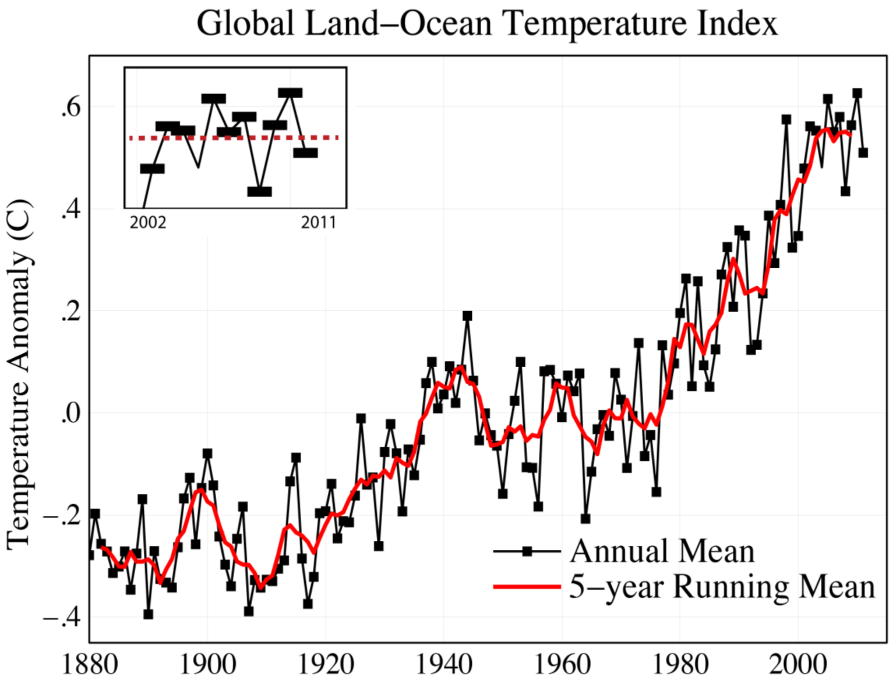


Fig. 7: Global land-ocean temperature index (data.giss.nasa.gov/gistemp/graphs_v3)

- The imbalance of the last decade heat has gone into deep oceans
- If climate forcing in 2050 reaches 4.5 W/m^2, what consequences might be expected?

Global Damage Due to CO_2 Emissions

- Global Social Cost of Carbon (GSCC) is 158 \$/tCO_2
- Global emission 33 Gt CO_2/y
- Global damage:

158\$/tCO2 x 33 Gt CO_2/y = 5-6 trillion \$/y

1/10 of the global GDP (69 trillion \$/y)

Trillion = 10^{12}

Global damage due to CO_2 at least 5-6 trillion \$/y!!

Global Damage Due to Human Unsustainable Practice

- CO_2 emission – global warming with unknown consequences 1/10 GDP
- NO_x emission – eutrophication, smog formation, ozone depletion, also global warming and biodiversity loss (damage even higher than by CO_2) >1/10 GDP
- Biodiversity loss – irreversible due to the extinction of species (extinction rate is up to 140,000 species per year) ?/10 GDP

Net GDP (€/y) = GDP – Eco-loss = GDP – GDP/2 = GDP/2

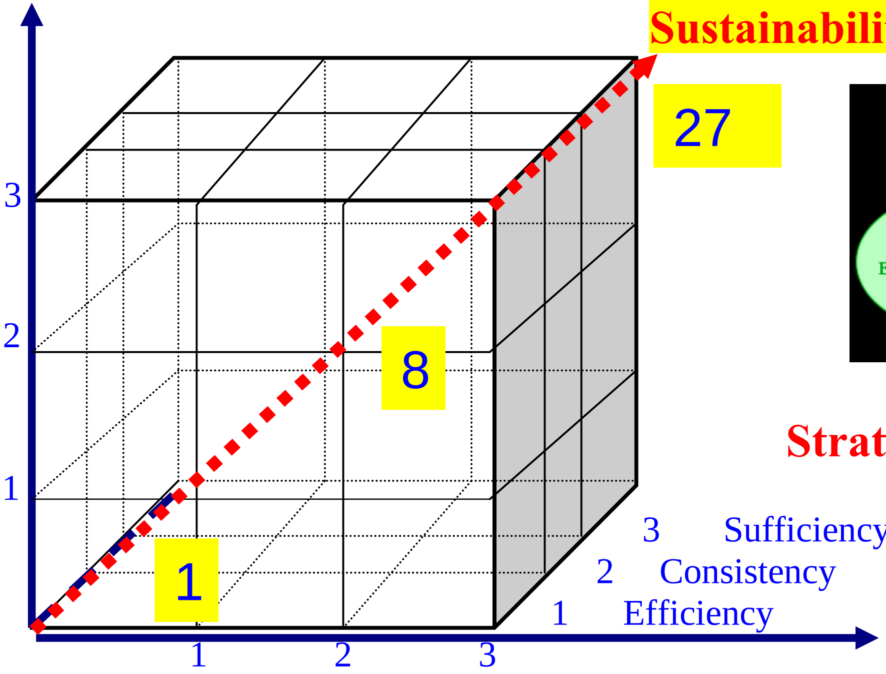
Conclusion: Global BDP is significantly overestimated!

Stagnation when $(\Delta GDP - \Delta Eco\text{-}loss)<0$

Sustainable development considerably improves global economics!

1.3 Sustainable Development and 3x3x3 Matrix of Sustainability

M. F. Jischa, Chem. Eng. Technol. 21, 1998



Nature

Eco-centric 3

Expanded-anthropozentric 2

Narrow anthropozentric 1

Sustainability

27

8

1

Strategies

3 Sufficiency

2 Consistency

1 Efficiency

1 Just Reward for Work

2 Respect for Private Property

3 Fair Distribution of Goods

Principle of Justice, Economics, Etics

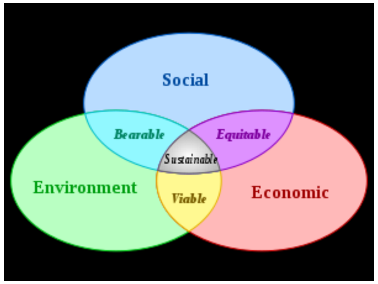


Figure 8: Diagonal as a measure of sustainability

Source: M. F. Jischa, Chem. Eng. Technol. 21, 1998

Sustainable Development: Blue Map – New Scenario for CO_2 Emissions

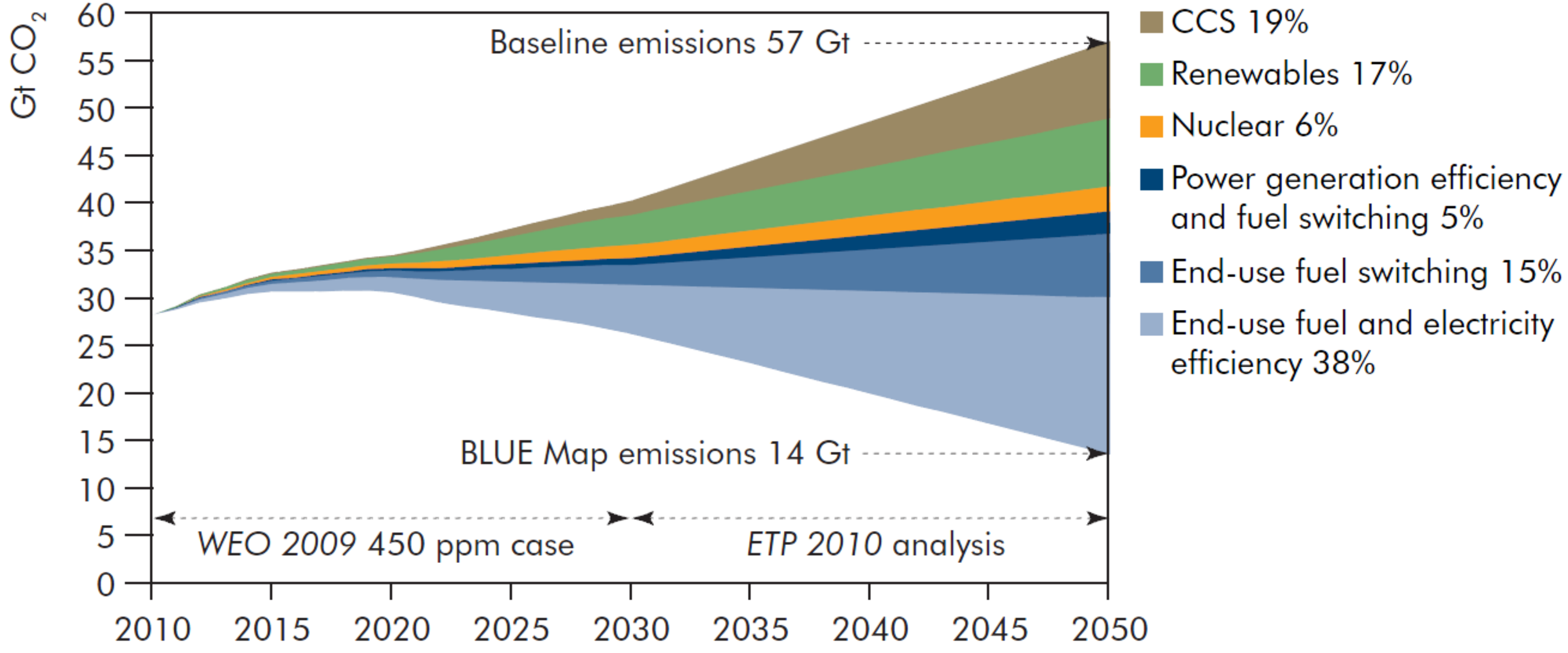


Fig. 9: Blue Map scenario and key technologies for reducing CO2 emissions

OECD/IEA. Energy Technology Perspectives 2010, Scenarios & Strategies to 2050, http://www.iea.org/techno/etp/etp10/English.pdf

Note: renewables mostly solar and wind, others hydro, biomass and waste, geothermal, and oceanic

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2. Holistic Design Methodology: LCA-Based System Synthesis

Synthesis is the **automatic generation** of **design alternatives** and the **selection of the better ones**

A. W. Westerberg, 1991

1. Holistic systems approach
2. System boundaries expanded to the synthesis of whole supply-chains and their networks comprising of sustainable alternatives
3. Automatic flowsheet synthesizer, e.g. MIPSYN, CAPE concepts and tool integration
4. Multiobjective LCA-based system synthesis considering:
   - direct (burdening) and
   - indirect (unburdening) environmental impacts

2.1 Holistic Systems Approach

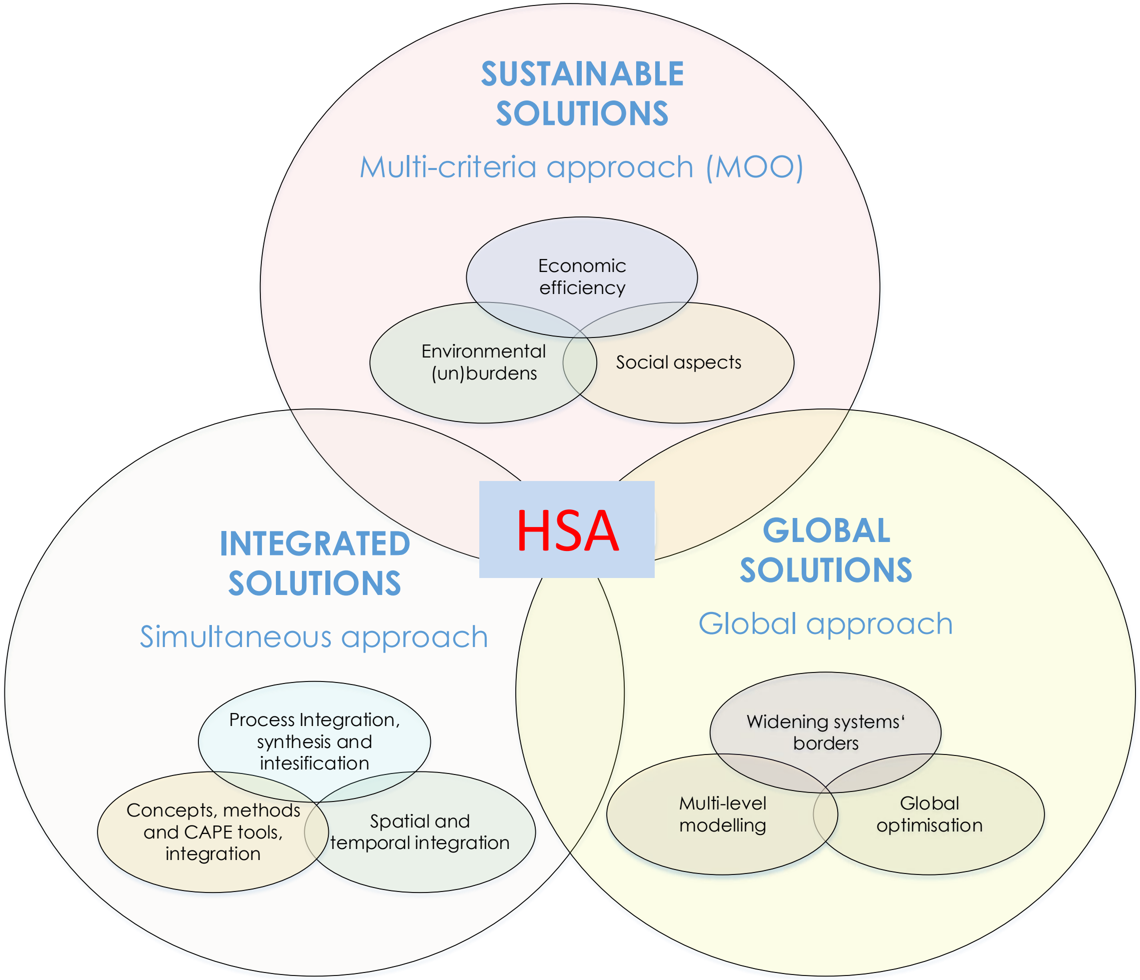

Fig. 10: Elements of the holistic systems approach

2.2 Creative Principles in Mathematics

But the
creative principle
resides in
mathematics.
In a certain sense,
therefore, I hold true
that pure thought can
grasp reality, as the
ancients dreamed.

Albert Einstein

Creative Principles of MP

Optimality	Competitive advantage
Feasibility	Constraints satisfied
Integrality	Simultaneous considerations

Creative principles of MP enables:

- Creation of new knowledge and
- New innovative solutions

Study of solutions enables one to get new insights, e.g. simultaneous Heat Integration and process flowsheet optimization also reduces raw material usage.

(Lang, Biegler, Grossmann, 1988)

2.3 Superstructure Approach for Systems Synthesis

1. Generation of a superstructure composed of different alternatives:
    - Reaction networks
    - Separation networks
    - Heat exchanger networks
    - Process schemes, etc.
2. Formulation of a mixed-integer nonlinear programming (MINLP) model
3. Solution by a suitable MINLP algorithm (OA/ER, General Benders Decomposition, Extended Cutting Plane..)

MINLP Model Formulation for Different Levels of Innovations:

$$
\begin{array}{llll}
\text{a)} & \max & z = c^{\mathrm{T}}y + f(x) - e(x) & \\
\text{b)} & \text{s.t} & h_i(x) = 0 & \\
\text{c)} & & g_i(x) \le 0 & \left.\right\} \forall i \in Subsystems \\
\text{d)} & & B_i y + C_i x \le b_i &
\end{array}
$$

$$x \in X = \{x \in R^n : x^{\mathrm{LO}} \le x \le x^{\mathrm{UP}}\}$$

$$y \in Y = \{0,1\}^m$$

a) Objective function as a real-world economic function (cost benefit approach):

Max Profit = Production income - Raw material cost - Utility cost

- Investment cost – Environmental loss

b) Equality constraints: mass and energy balances, design equations

c) Inequality constraints: product specifications, operational, environmental and feasibility constraints

d) Logical disjunctive constraints for selection of sustainable alternatives

2.4 Challenges Related to the Manifolds Nature of the Synthesis Problems

Features:	Approach:
Many complex interactions	Simultaneous
Discrete and continuous decisions	MINLP
Uncertainty	Flexible multiperiod
Dynamic systems	MIDNLP, multiperiod
Rule-based decisions	Logic-based
Multicriterial	Multiobjective LCA-based

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3.1 Simultaneous vs. Sequential Strategy Methanol Example Problem

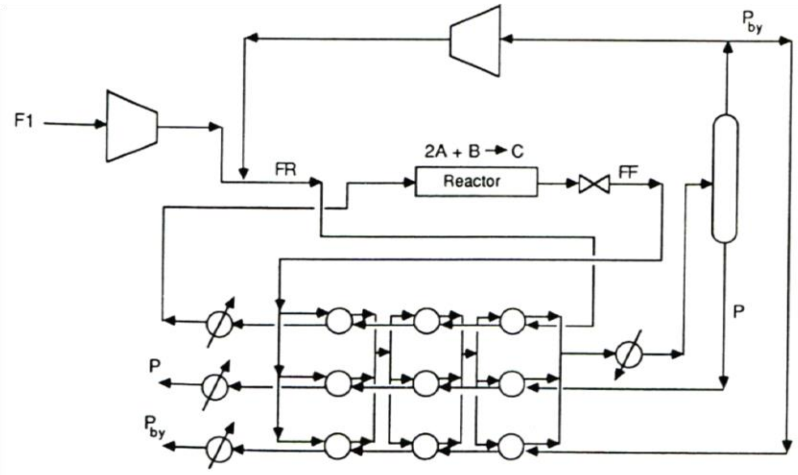


Figure 11: Methanol process and HEN superstructure

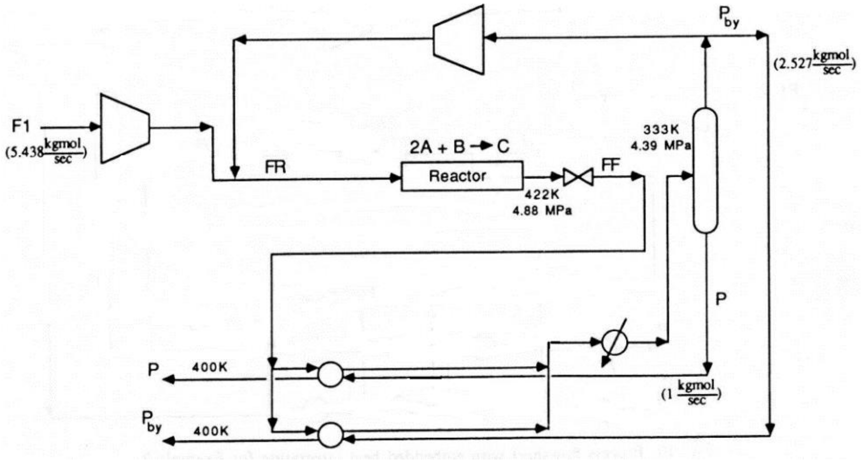


Figure 12: Optimal process scheme with HI HEN

Process synthesis and:

• sequential HEN synthesis:	- 1,192,000 $/yr (loss!)
• simultaneous HI by Duran-Grossmann's model:	- 292,000$ $/yr (loss!)
• simultaneous HEN synthesis by Yee's model:	
• Yee, Grossmann, Kravanja (1990)	1,845,000 $/yr (profit!).
• Kravanja and Grossmann (1994)	**2,613,000** $/yr (**profit**!)

3.2 Simultaneous vs. Sequential Strategy
Scope of HI in Total Sites

Process level: heat exchange occurs directly between the hot and cold streams

Total Site (TS) level: where mostly indirect heat exchange is performed between hot and cold streams via an intermediate utility

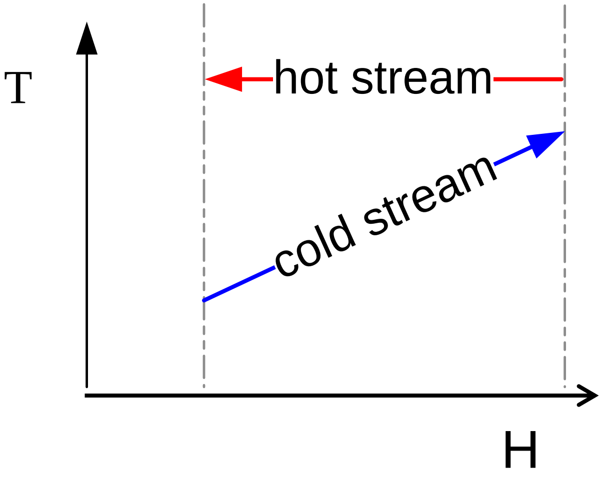


Figure 13: HI at process level

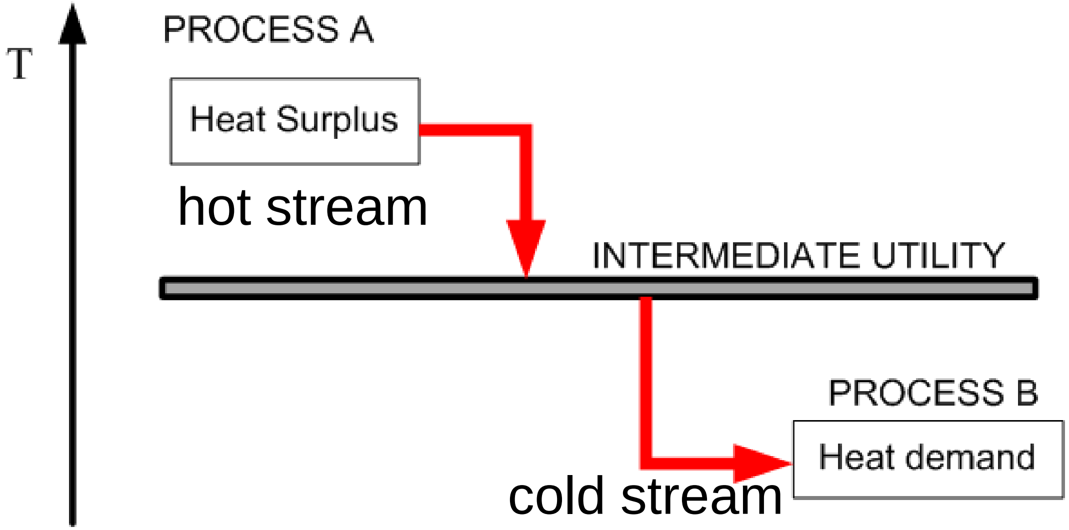
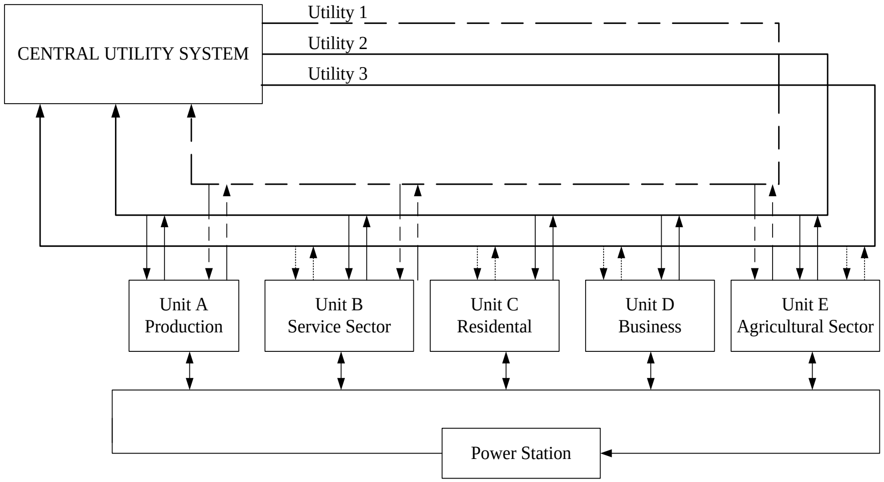


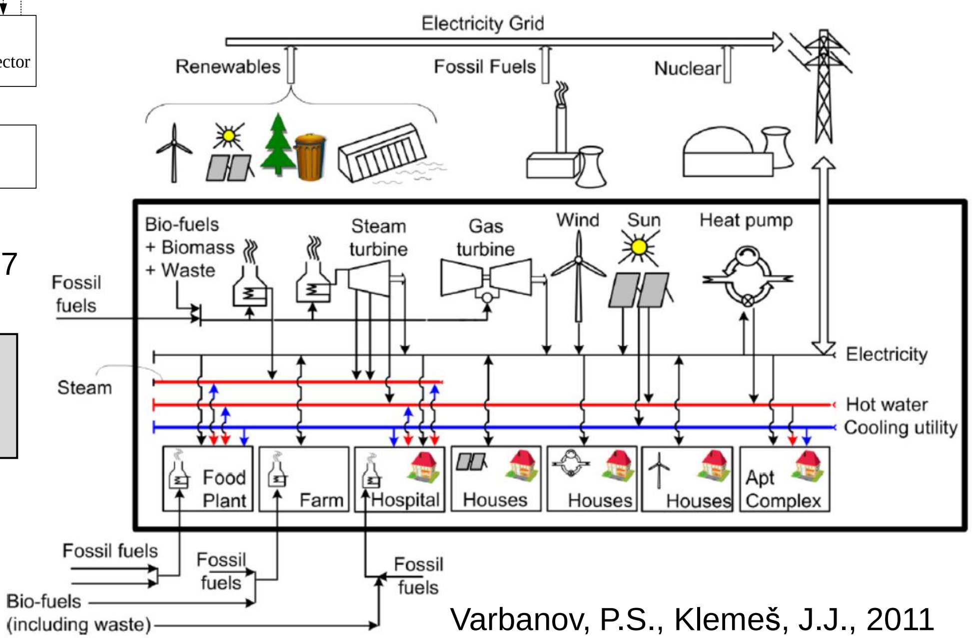
Figure 14: HI at Total Site level

Total Site



Dhole and Linnhoff, 1993; Raissi, 1994; Klemeš et al., 1997
Perry, Klemeš, Bulatov, 2008 - LIES

Figure 15: Scheme of Total Site
Extended form Perry et al. (2008)



Varbanov, P.S., Klemeš, J.J., 2011

Figure 16: Extended for renewables
Source: Klemeš et al., CERD, 2013

Simultaneous Strategy

Heat exchange matches on process level and Total Site considering intermediate utility (**indirect process-to-process heat exchange)** are included in each stage

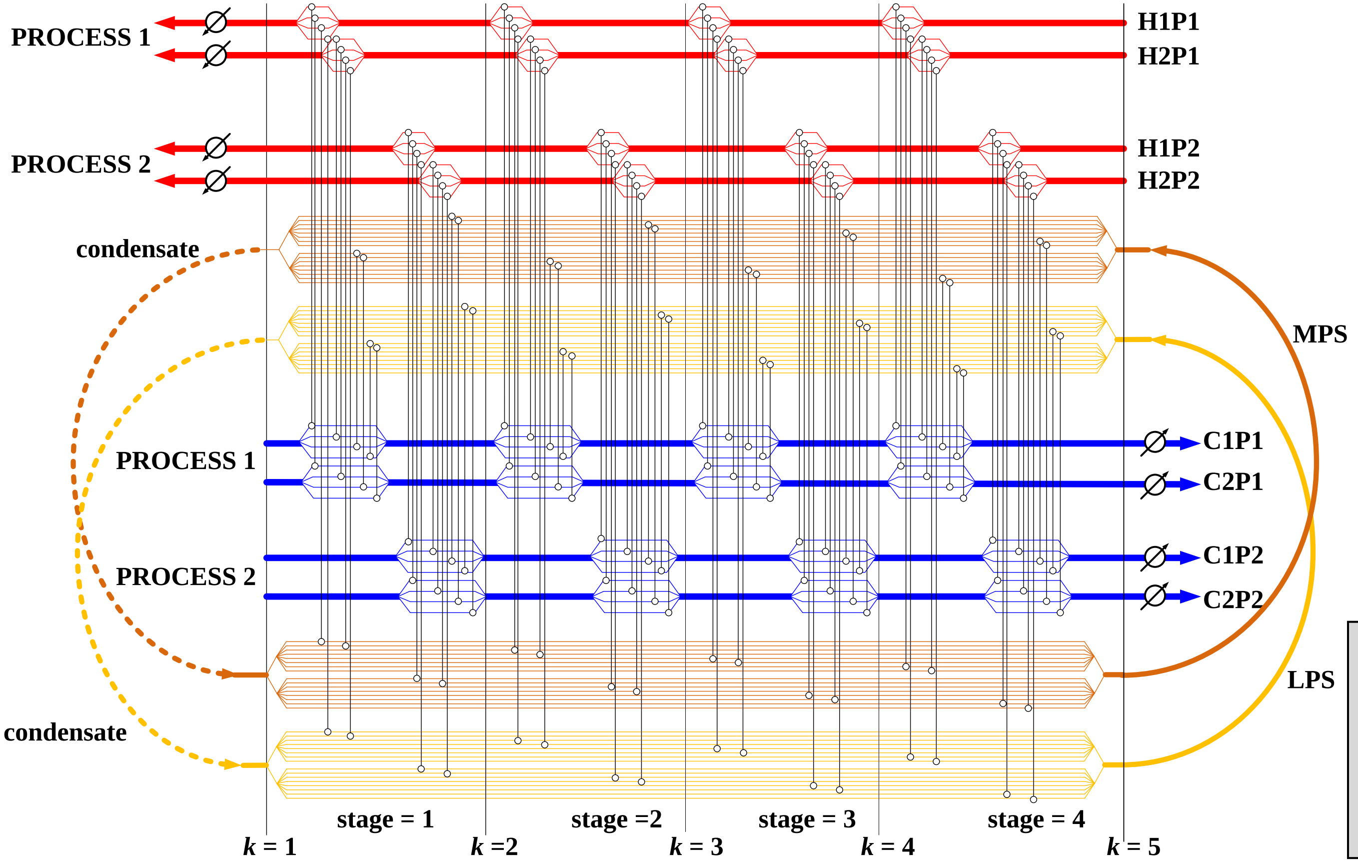


Figure 17: General superstructure - simultaneous strategy

Issues Matters

Nemet, Klemeš, Kravanja, 2014 DOI: 10.1016/j.compchemeng.2014.07.004

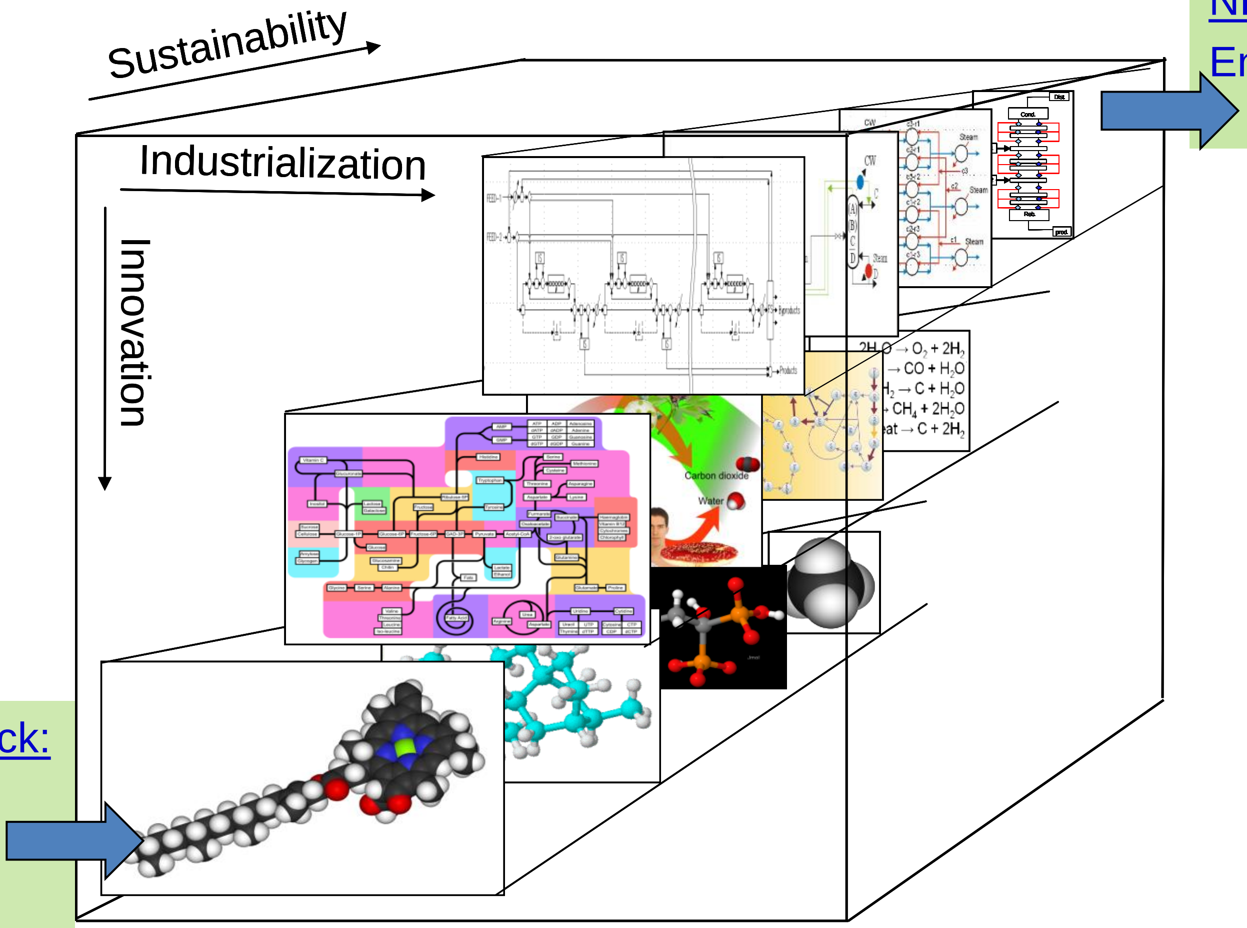
STRATEGY:	SAVINGS in NPV
Simultaneous Strategy vs. Sequential Strategy	64 %
Pressure level optimization	33 %
Future forecasted utility prices	18 %

Other considerations:

- Pipeline investment ~up to 34.2 % of the total investment.
- Heat losses ~ can be up to 44.8 % at fixed utility pressure levels when no preheating was considered
- Pressure drops simultaneously with the evaluation of pipe diameters ~ pressure drops can be quite high (even 4 bar)
- Preheating of fresh water due to unrecovered condensations it significantly reduces *ENPV* by 11.0 %, the hot utility consumption increased by 33.2 %

3.3 Expanding the Synthesis to the Whole (Bio)-chemical Supply Chain

Kravanja, CACE 2010



NEW Products:
Environmentaly benign

NEW Feedstock:
- Recycled
- Waste
- Renewable

Fig. 18: Simplified (bio)-chemical supply chain.

Expanding the Synthesis to Energy Supply Chain

Kravanja, 2009

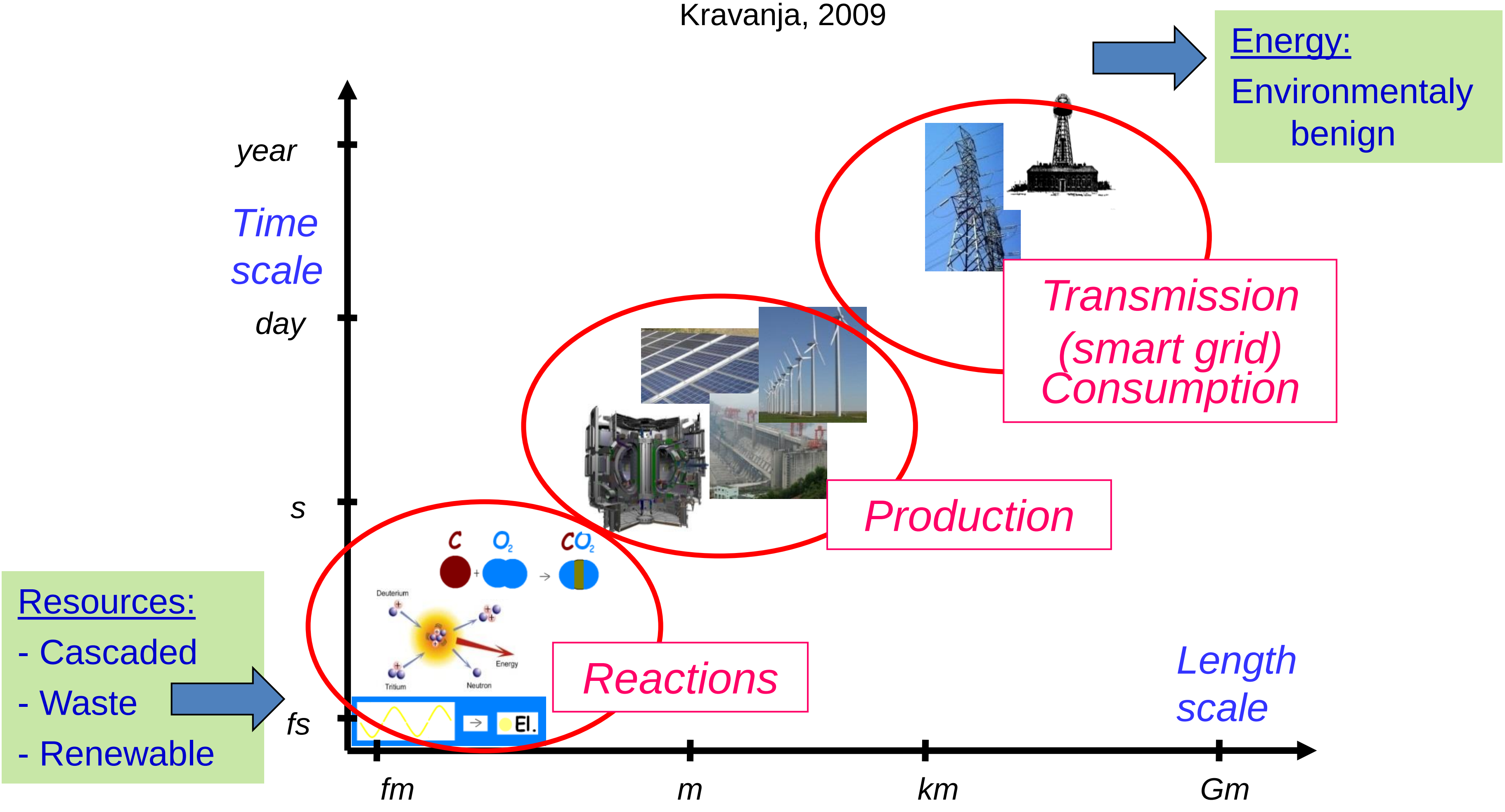
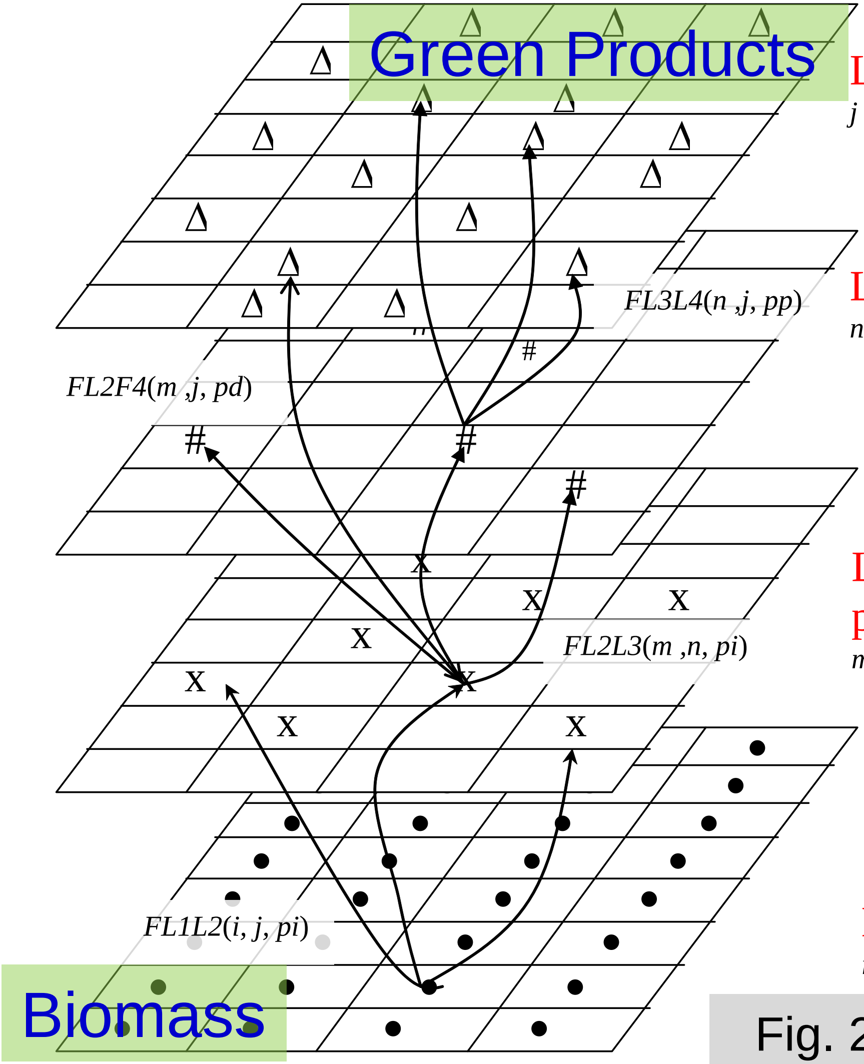


Fig. 19: Achieving global solutions through the integrated energy supply chain

Expanding the Synthesis to Regional Supply/Demand Renewable Networks

Čuček, Lam, Klemeš, Varbanov, Kravanja, 2010



Layer 4: Demand/ End users

j = demands

Layer 3: Production plants

n = plants

*y*L3 (n) = To determine the location of plants
*y*L3pt (*n*, *pp*, *t*) = for technologies selection

Layer 2: Collection and pretreatment processes

m = intermediate points

*y*L2 (*m*) = To determine the location of collection points and also the pretreatment processes : drying/ compaction/ densification

Layer 1: Agricultural supply

i = zones

Fig. 20: SDRN superstructure

Simultaneous

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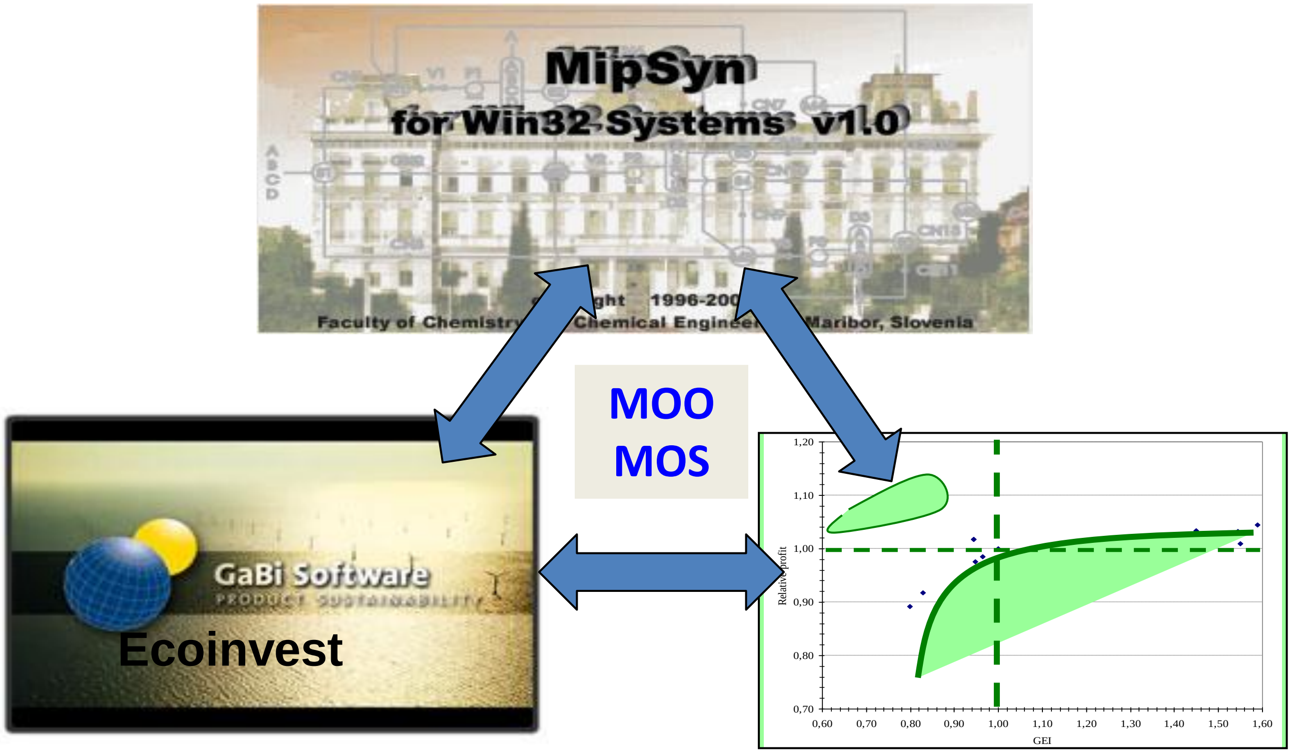
4.1 Tools Integration:
LCA-based Synthesizer

Synthesizer



MOO
MOS

LCA, Database

Graphical output

Fig. 21: LCA-based synthesizer MIPSYN

4.2 Concepts Integration: Combining Pinch Analysis and Mathematical Programming

Jiří Jaromír Klemeš & Zdravko Kravanja, COCHE, 2013

	Pinch approach	MP approach	Combined approach
Guiding principle	Physical insights Clear concepts	Numerical Mathematics	Narrowing the searching space
Embedded principles	Consideration of physical laws	Optimality, feasibility, integrality	Both principles are considered
A single criterion	Mainly technological criteria	Mainly economical criterion	Appropriate economic trade-offs
Multi-criteria consideration	Difficult to express graphically	MOO performed for several criteria	Multi-criteria can be considered
Degrees of freedom	Difficult to express graphically	Handles a large number of variables	Large problems can be solved
Data collection and verification	The physical inside makes the checking easier	A possibility to apply data reconciliation algorithms	Combination can be very beneficial

Opportunities of Employing a Combined PA/MP Approach

	Pinch approach	MP approach	Combined approach
Uncertain data and parameters	Limited number of uncertain parameters and limited flexibility	A reasonable number of parameters, reasonable flexibility	Feasible, realistic and flexible solutions can be obtained
Approach strategy	Can eliminate easily physically non feasible solutions	Simultaneous, fully integrated solutions	By both strategies in a sequence fully integrated solutions
Problem formulation	Graphical and algorithmic and form – easily understandable	Usually Equation-Oriented (EO) mathematical form.	Hybrid model enabling solving larger-scale problems
Easiness of formulation	Straightforward and mostly easy	Could be very complicated	Pinch is beneficial in the first step followed by MP
Easiness of problem reformulation	Very easy when supported by PTA	Many scenarios can be routinely performed	Pinch is again beneficial in the first step followed by MP

Opportunities of Employing a Combined PA/MP Approach

	Pinch approach	MP approach	Combined approach
Optimality of solutions	Global optimal targets can be indicated based on the thermodynamics	Locally optimal techniques and solutions	Pinch concept can guide MP solutions close to global optima
Comprehension of solution	Straightforward with graphical methods and PTA New insights	Not easy to be interpreted. New insights	Combined graphical interfaces to mimic MP solutions
Knowledge needed	Seems basic engineering, however needs a process expert	Advanced knowledge, both engineering and MP	Experienced Process engineer guaranties realistic solution for both approaches
Robustness	Robust, which is important for engineering practice	LPs and MILPs robust, NLPs and MINLPs need good initialization	Overall robustness in solving large-scale problems is improved by the synergy
Current industrial acceptance	High, easily understandable to engineers on the ground	So far lower, boosted by engineering friendly interface	Could foster the acceptance of MP in process and other industries

Achieving Energy Savings in Total Sites

Two widely used methodologies for energy consumption targeting: Pinch Analysis and Mathematical Programming

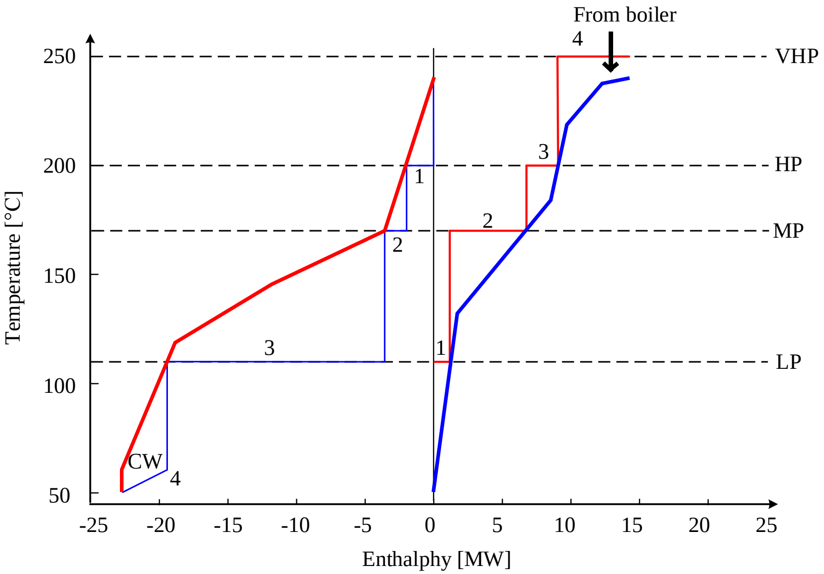


Fig. 22: Total Site Profiles and intermediate utility, (from Klemeš et al., 2010)

$$\max_{x,y} P = (c^{\mathrm{T}} y + f(x))$$

$$\text{s.t.} \qquad h_{l,s}(x,y) = 0 \qquad \forall l \in L, s \in S$$

$$g_{l,s}(x,y) \le 0 \qquad (\text{F-MINLP}_i)_f$$

$$DRFP_f(x,y)_{P_{\max}} \le \varepsilon_{if}, \qquad \forall i \in I, f \in F$$

$$(x^{LO} x \le x^{UP}) \in X \subset \mathrm{R}^n, \quad y = \{0,1\}^m$$

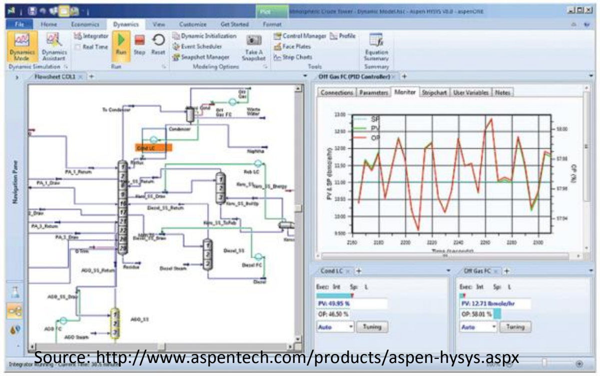
$$\varepsilon_{if} = \varepsilon_{i-1,f} - \Delta\varepsilon_f$$

Fig. 23: Heat integration solutions from mathematical model

Tools Integration for Retrofit of Total Site

Lidija Čuček & Zdravko Kravanja, PRES 2014

I. Process Simulator Data Acquisition

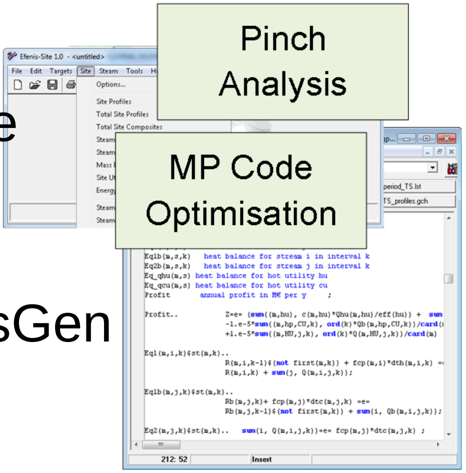

Source: http://www.aspentech.com/products/aspen-hysys.aspx

Aspen, Hysis

II. Combined Pinch/MP Optimization

Efenis-Site

TransGen

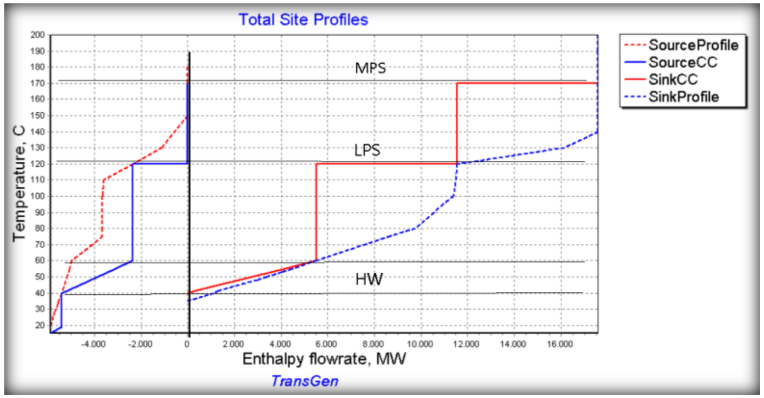


Pinch Analysis

MP Code Optimisation

```
Eq1b(m,s,k)   heat balance for stream i in interval k
Eq2b(m,s,k)   heat balance for stream j in interval k
Eq_qhu(m,s) heat balance for hot utility hu
Eq_qcu(m,s) heat balance for hot utility cu
Profit       annual profit in M€ per y     ;

Profit..          Z=e= (sum((m,hu), c(m,hu)*Qhu(m,hu)/eff(hu)) +  sum
                  -1.e-5*sum((m,hp,CU,k), ord(k)*Qb(m,hp,CU,k))/card(
                  +1.e-5*sum((m,HU,j,k), ord(k)*Q(m,HU,j,k))/card(m)

Eq1(m,i,k)$st(m,k)..
                  R(m,i,k-1)$(not first(m,k)) + fcp(m,i)*dth(m,i,k) =
                  R(m,i,k) + sum(j, Q(m,i,j,k));

Eq1b(m,j,k)$st(m,k)..
                  Rb(m,j,k)+ fcp(m,j)*dtc(m,j,k) =e=
                  Rb(m,j,k-1)$(not first(m,k)) + sum(i, Qb(m,i,j,k));

Eq2(m,j,k)$st(m,k)..   sum(i, Q(m,i,j,k))=e= fcp(m,j)*dtc(m,j,k) ;
```

III. Graphical and Numerical Output



GAMS gdx and chard files

Fig. 24: Three-level tool integration

Tools Integration

- Incentives for Sustainable Development
- LCA-based Mathematical Programming for Sustainable System Synthesis
- Expanding Systems Boundaries
- Tools and Concepts Integration
- New Concept Considering Burdening and Unburdening Effects on Environment in Multiobjective Optimization:
  - Total Footprints,
  - Total Sustainability Index, and
  - Eco-Profit and Total Profit
- Synthesis Applications of Renewables Integration and Bioenergy Production
- Conclusion

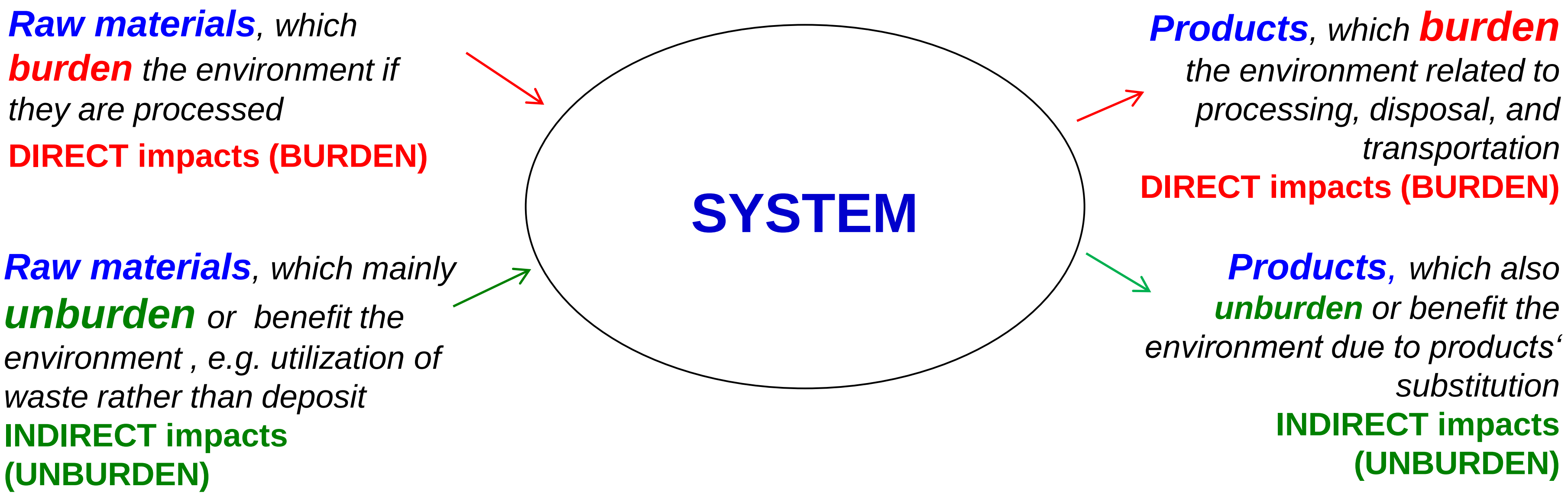
5. Multiobjective LCA-based System Synthesis

- Sustainability and especially environmental indicators defined on the LCA based principles
- Incomplete measurements for sustainability is one of the major limitations of LCA methodology
- Consequences: poor or even wrong solutions and decisions!

More advanced concept and measurements are needed

Besides the direct (burdening), also indirect (unburdening) effects caused by system‘s substitution have to be considered

LCA-based System Synthesis
New Concept: Direct and Indirect Effects



***Raw materials**, which **burden** the environment if they are processed*

DIRECT impacts (BURDEN)

***Raw materials**, which mainly **unburden** or benefit the environment , e.g. utilization of waste rather than deposit*

INDIRECT impacts (UNBURDEN)

SYSTEM

***Products**, which **burden** the environment related to processing, disposal, and transportation*

DIRECT impacts (BURDEN)

***Products**, which also **unburden** or benefit the environment due to products‘ substitution*

INDIRECT impacts (UNBURDEN)

The DIRECT effects of systems on the environment represent direct burden of the systems due to the extraction of resources, materials production, use, maintenance, recycling and/or disposal including all transportation steps.

The INDIRECT effects are those sets of impacts that indirectly unburden or benefit the environment when waste is utilized instead of being deposited or environmentally benign raw-materials, products or services are used instead of harmful ones.

TOTAL effects = DIRECT + INDIRECT effects

LCA-based Synthesis Approach
Direct vs. Total Environmental Effects

Direct Effects:

1. Footprints
2. Sustainability Index
3. Eco-cost
   (Vogtländer et al., 2010)

+ Indirect effects

Total Effects: (Kravanja, COCHE, 2012)

1. Total Footprints
   (Čuček, Varbanov, Klemeš, Kravanja, Energy, 2012)
2. Total Sustainability Index
   (Kravanja, Čuček, APEN, 2013)
3. Eco-profit and Total Profit
   (Čuček, R. Drobež, B. Pahor, Z. Kravanja, CCE, 2012)

Towards Non-trade-off Solutions

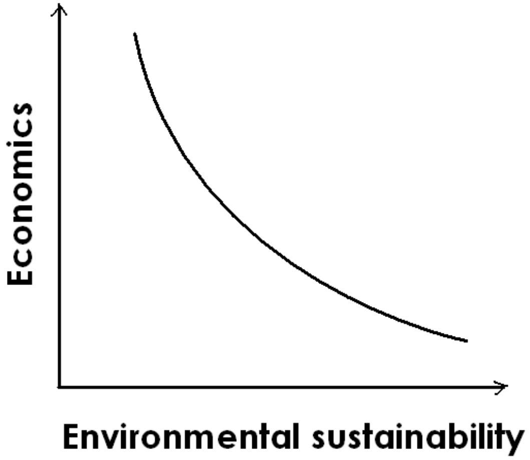


Fig.25. Pareto curve

General opinion: There is an opposition between economics and environmental sustainability

- This is not always true as some alternatives can have synergistic effects on both the environment and the economics.
- Non-trade-off solutions can thus be obtained.

- Incentives for Sustainable Development
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    - Total Footprints,
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    - Eco-Profit and Total Profit
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- Conclusion

5.1.1 Definition and Normalization of Footprints

- Footprints cannot be easily compared since they can have different measures, units, and qualities

- Footprints of studied alternatives are normalized, e.g. by the values obtained at the maximal profit or from some base-case design:

Direct relative footprint

Total relative footprint

$$DRFP = \frac{FP^{\mathrm{d}}}{FP^{\mathrm{d0}}}$$

$$TRFP = \frac{FP^{\mathrm{d}} + \boxed{FP^{ind}}}{FP^{\mathrm{d0}}} = \frac{FP^{\mathrm{t}}}{FP^{\mathrm{d0}}}$$

Direct Footprint at the maximal profit

Footprint-based MINLP Synthesis

Two-step multi-objective superstructural MINLP approach:

MINLP step I:

Economic-based synthesis where different footprints are obtained by the maximization of profit from a given basic superstructure:

$$P^0 \text{ and } FP_f^{\mathrm{d},0}, \quad \forall f \in F$$

Reference point

MINLP step II:

The superstructure is augmented by sustainable alternatives and the ε-constraint method is applied for each relative footprint *f* є *F*:

$$P_k,\ FP_{f,k}^{\mathrm{d}} \text{ and } FP_{f,k}^{\mathrm{ind}}, \forall f \in F,\ k \in F$$

Multi-objective Pareto solutions

5.1.2 Direct Effects
Footprint–based MINLP

Small- and medium-sized supply-networks

Footprints: carbon, water, non-renewable energy, emission (water, air, soil), food vs. fuel

Direct relative footprint

$$RFP = \frac{FP^{\mathrm{d}}}{FP^{\mathrm{d},0}}$$

Direct footprint at the maximal profit

$$\max_{x,y} P = (c^{\mathrm{T}} y + f(x))$$

s.t. $h_{l,s}(x,y) = 0 \qquad \forall l \in L, s \in S$

$g_{l,s}(x,y) \le 0 \qquad (\text{F-MINLP}_i)_f$

$DRFP_f(x,y)_{P_{\max}} \le \varepsilon_{if}, \qquad \forall i \in I, f \in F$

$(x^{LO} x \le x^{UP}) \in X \subset \mathrm{R}^n, \quad y = \{0,1\}^m$

$\varepsilon_{if} = \varepsilon_{i-1,f} - \Delta\varepsilon_f$

Loop around Solve statement in GAMS

Direct effects
Footprint-based Pareto Solutions, MINLP II

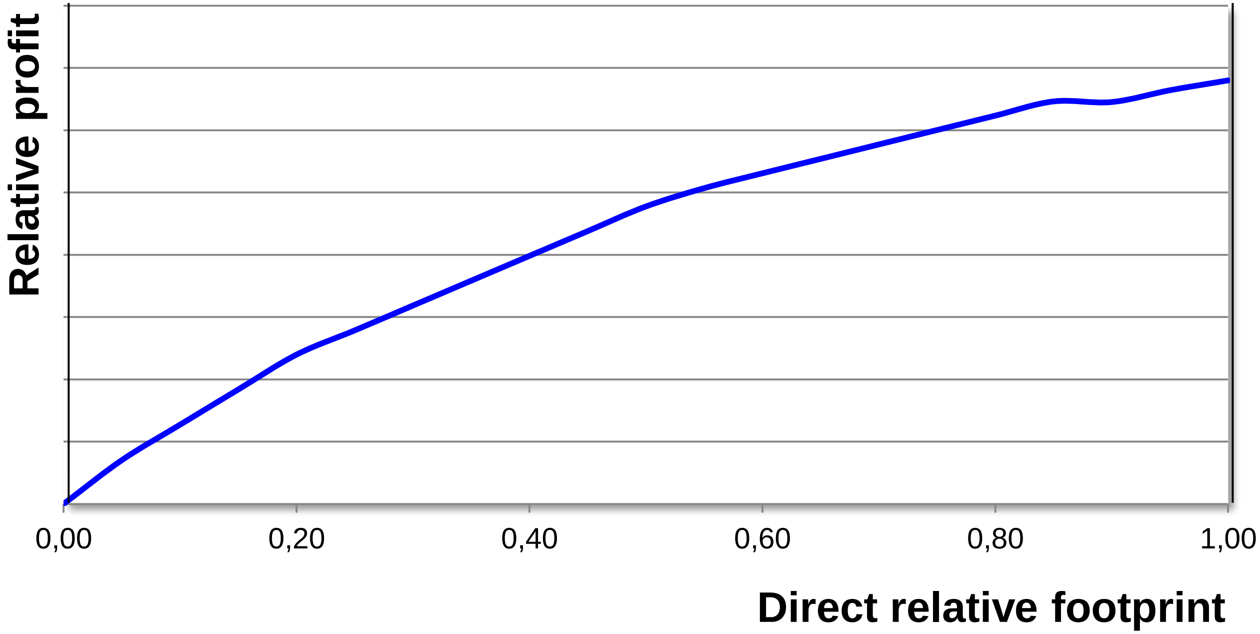


Fig.26: Profit vs. Direct footprint

5.1.2 Total Effects
Total Footprint–based MINLP II

Čuček, Varbanov, Klemeš, Kravanja, Energy, 2012

$$\max_{x,y} P = (c^{\mathrm{T}} y + f(x))$$

$$\text{s.t.} \quad h_{l,s}(x,y) = 0 \qquad \forall l \in L, s \in S$$

$$y_{l,s}(x,y) \le 0 \qquad (\text{F-MINLP}_i)$$

$$TRFP_f(x,y)_{P_{\max}} \le \varepsilon_{if} \qquad \forall i \in I, f \in F$$

$$(x^{LO} x \le x^{UP}) \in X \subset \mathrm{R}^n, \quad y = \{0,1\}^m$$

$$\varepsilon_{if} = \varepsilon_{i-1,f} + \Delta\varepsilon_f$$

$$TRFP = \frac{FP^{\mathrm{d}} + FP^{ind}}{FP^{\mathrm{d0}}} = \frac{FP^{\mathrm{t}}}{FP^{\mathrm{d0}}}$$

Total Effects: Total Footprint-based Pareto Solutions, MINLP II

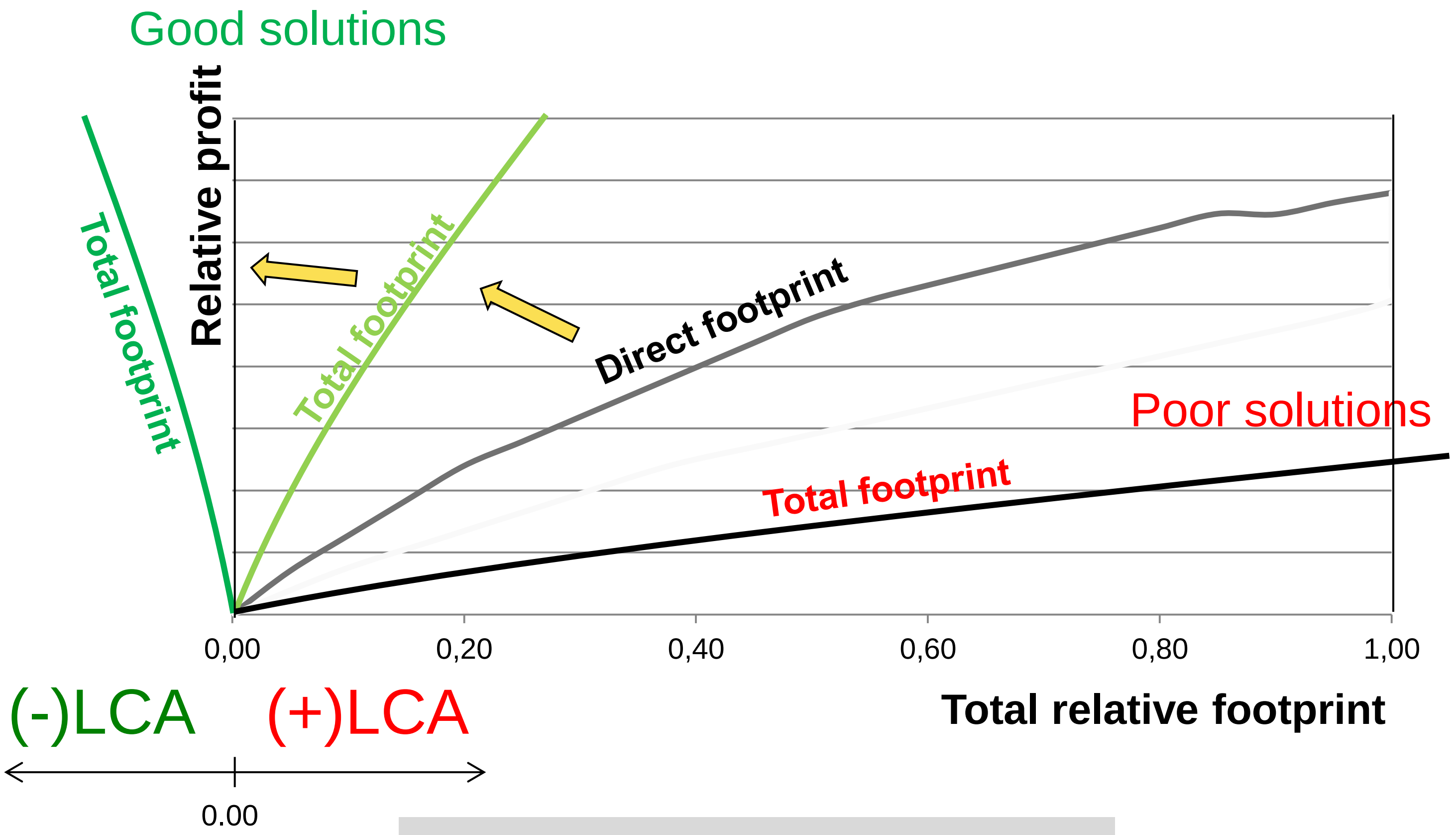
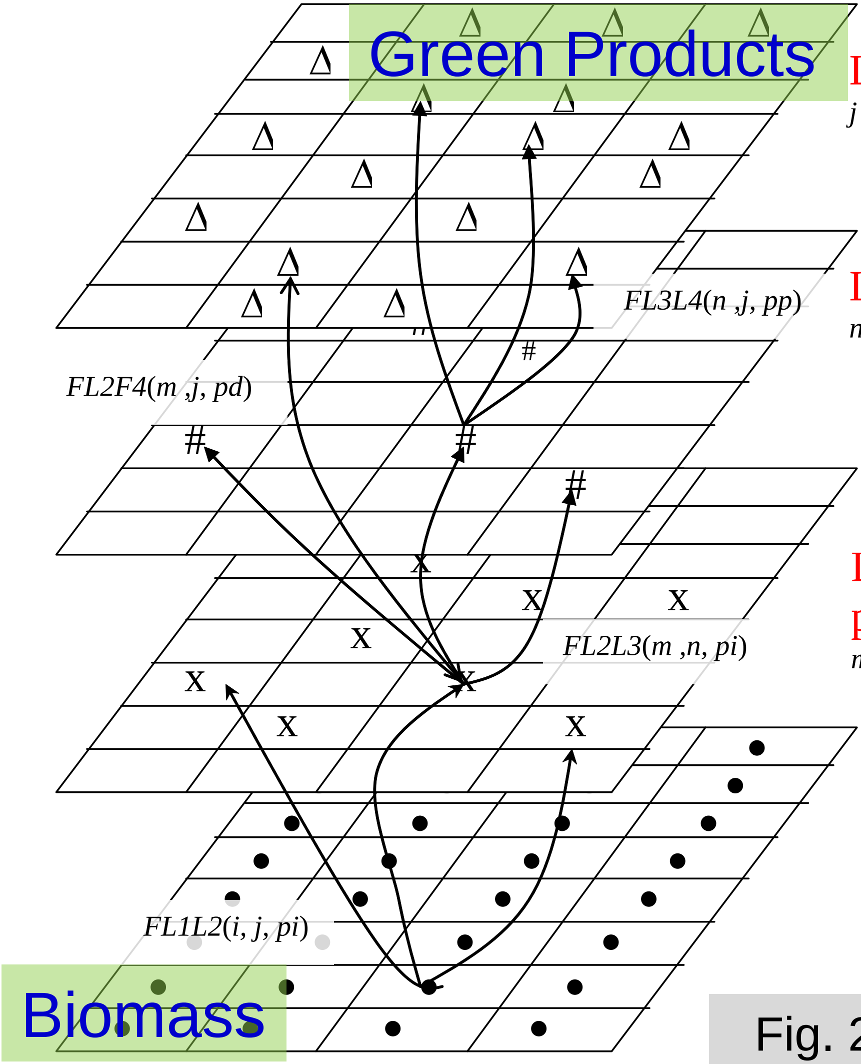


Fig. 27: Profit vs. Total footprint

5.1.3 Case Study: Biomass Supply Chain and Total Footprints

Čuček, Varbanov, Klemeš, Kravanja, Energy, 2012



Layer 4: Demand/ End users

j = demands

Layer 3: Production plants

n = plants

*y*L3 (n) = To determine the location of plants
*y*L3pt (*n*, *pp*, *t*) = for technologies selection

Layer 2: Collection and pretreatment processes

m = intermediate points

*y*L2 (*m*) = To determine the location of collection points and also the pretreatment processes : drying/ compaction/ densification

Layer 1: Agricultural supply

i = zones

Fig. 28: SDRN superstructure

Biomass Supply Chain – Footprints

Environmental footprints *f* ε *F*:

- CFP (Carbon footprint) – amount of CO_2 and other greenhouse gases emitted over the full life-cycle of a process or product
- EFP (Energy footprint) – the demand for non-renewable energy resources
- WFP (Water footprint) – the total volume of direct and indirect freshwater used
- LFP (Agricultural land footprint) – the agricultural land area used for growing biomass
- WPFP (Water pollution footprint) – the amount of substances emitted to water

Social footprint

- FEFP (Food-to-energy footprint) – relates the usage of food intended biomass for the production of energy

Demonstration Case Study

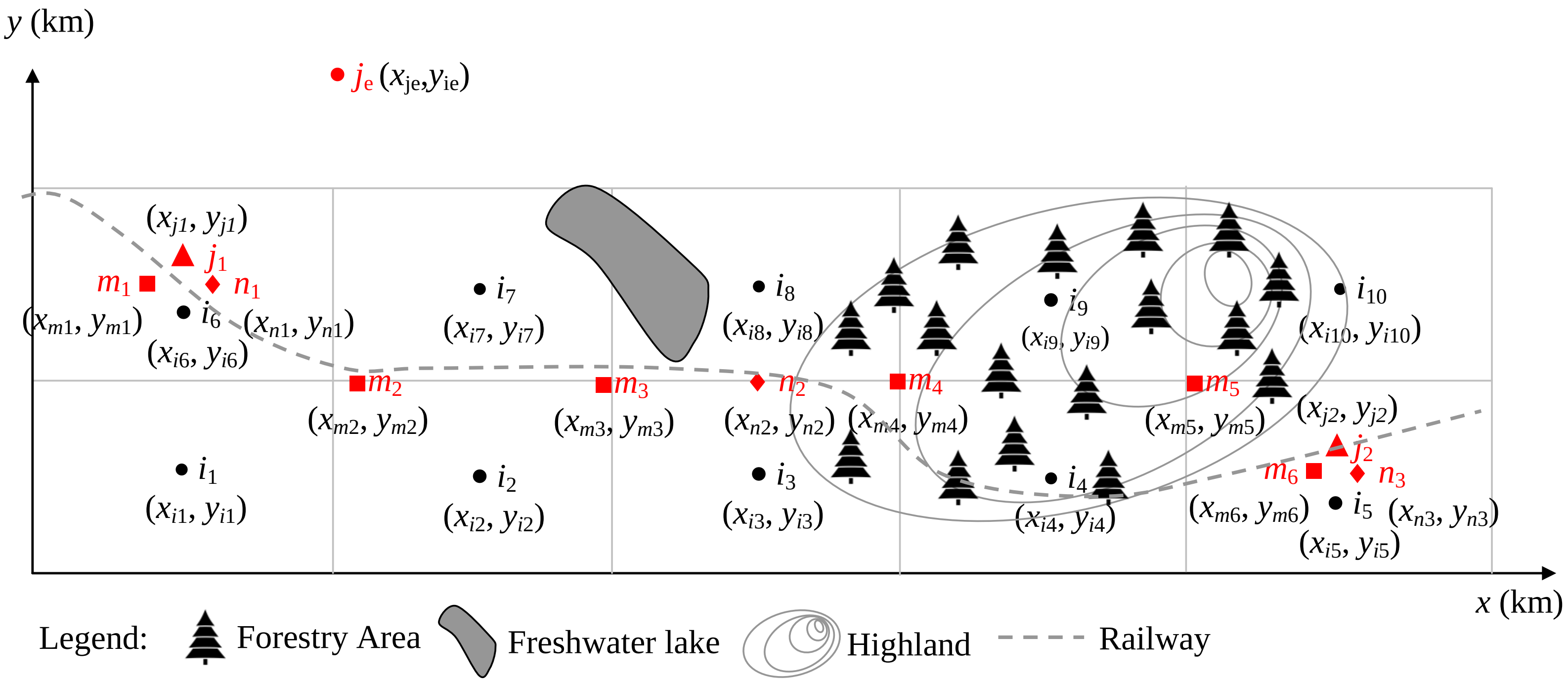


Fig. 29: The supply-network structure of the demonstrated case study

Čuček, Lam, Klemeš, Varbanov, Kravanja, CTEP 2010

Biomass Supply/Demand Renewable Networks

- Raw materials included on the given area:
  corn, corn stover, MSW, wood chips, manure and timber

- Considered technological options:
  - The dry-grind process (corn)
  - Diluted acid pre-treatment (corn stover)
  - Gasification/fermentation (wood chips)
  - Anaerobic co-digestion (biomass waste)
  - Incineration (MSW and lignocellulosic raw materials)
  - Sawing (timber)

- Products:
  electricity, heat, bioethanol, boards, digestate, DDGS

Footprints Obtained at MINLP-1

Table 1: Direct, Indirect and Total footprints for Biomass supply chain

	Direct footprints	Indirect footprints	Total footprints
CFP (t/(km^2·y))	117.65	-311.95	-194.3
WFP (t/(km^2·y))	376,500.75	-39,210.75	337,290
EFP (GJ/(km^2·y))	1,440.65	-4,906.72	-3,466.07
WPFP (t/(km^2·y))	12.02	-6.47	5.55
LFP (km^2/(km^2·y))	0.32	0	0.32
FEFP (-)	0.38	0	0.38

MINLP II: 2-D Projections of Direct Footprints

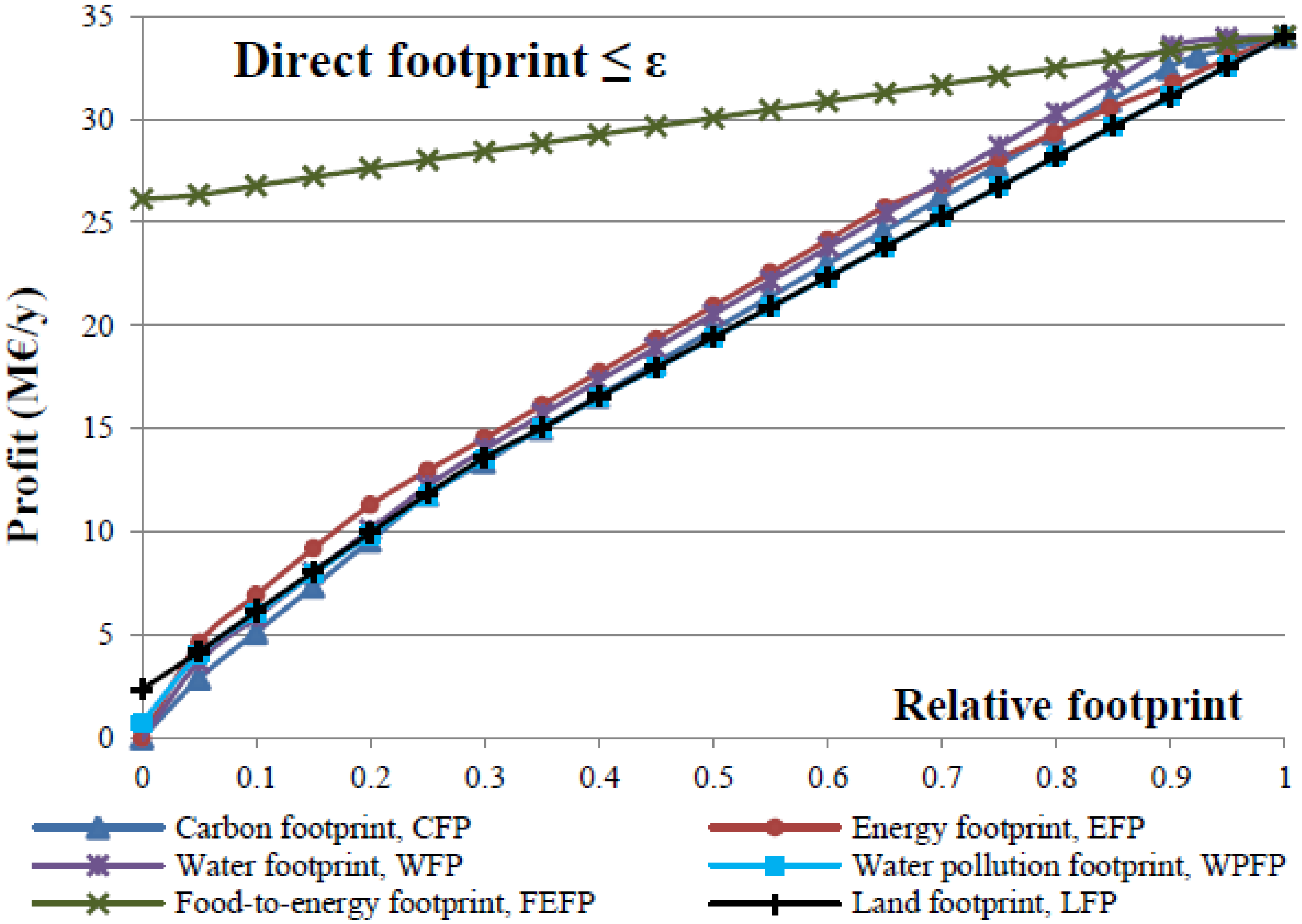


Fig. 30: Direct footprints for Biomass supply chain

2-D Projections of Total/Direct Footprints

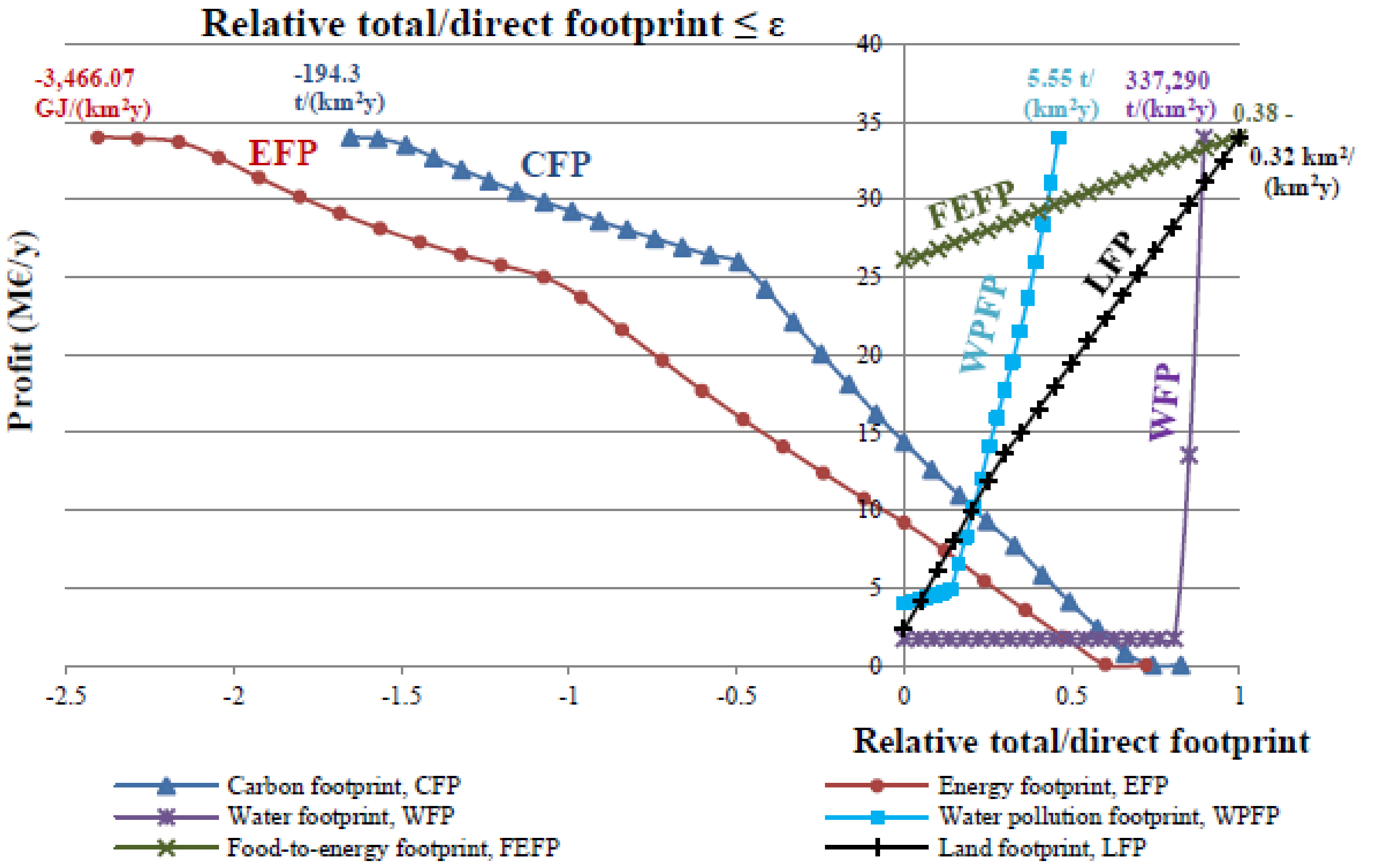


Fig. 31: Total/direct footprints for Biomass supply chain

Footprint-based Synthesis

ADVANTAGES

- For 2-D problems number of iterations increases linearly with the number of footprints
- 2-D multi-objective optimization for:
  - Any number of footprints
  - Medium- and larger-sized problems

PROBLEMS

- Footprints in 2-D projections are underestimated
- Higher-D problems needs large numbers of iterations, which cannot be applied to large-sized problems

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5.2.1 Definition and Normalization of Sustainability Index

- Economic, environmental and social indicators
  - Yearly profit (P) or the net present worth (NPW)
  - Environmental: resource usage and pollution indicators
  - Social: assessment is difficult
- Indicators are normalized, e.g. by the values from a given base case and
- Composed into Relative Sustainability Index:

$$RSI = \sum_{f \in F} w_f \cdot \frac{I_f}{I_f^0}$$

Conventional

New approach

Relative Direct Sustainability Index

RDSI (direct effects)

$$RDSI = \sum_{f \in F} w_f \cdot \frac{I_f^{\mathrm{d}}}{I_f^{\mathrm{d},0}}$$

Relative Total Sustainability Index

RTSI (direct + indirect effects)

$$RTSI = \sum_{f \in F} w_f \cdot \frac{I_f^{\mathrm{d}} + \boxed{I_f^{\mathrm{ind}}}}{I_f^{\mathrm{d},0}} = \sum_{f \in F} w_f \cdot \frac{I_f^{\mathrm{t}}}{I_f^{\mathrm{d},0}}$$

Since I_i^{ind} are negative, RTSI < RDSI

Total SI-based MINLP Synthesis

Two-step multiobjective superstructural MINLP approach:

MINLP Step I: **Economic-based** synthesis for basic process superstructure that comprises technological end economical alternatives

Base case solution

$$P^0 \text{ or } NPW^0,\ I_i^{\mathrm{d},0} \text{ and } I_i^{\mathrm{ind},0}\ \forall i \in I$$

Reference point

MINLP step II:

Multiobjective synthesis for superstructure**,** augmented by sustainable energy, environmental and other alternatives

Sustainable solution

$$P_k \text{ or } NPW_k,\ I_{i,k}^{\mathrm{d}} \text{ and } I_{i,k}^{\mathrm{ind}}\ \ \forall i \in I, k \in K$$

Total Effects
RTSI in ε-constrained MINLP II

Kravanja, Čuček, APEN, 2013

$$\max RP = (c^{\mathrm{T}} y + f(x)) / P^0$$

$$\text{s.t.}\quad \left.\begin{aligned} & h_l(x, y_{ls}) = 0 \\ & g_l(x, y_{ls}) \le 0 \\ & RTSI(x, y_{ls}) \le \boxed{\varepsilon_k} \end{aligned}\right\} \quad \forall l \in L, s \in S$$

$$x \in X = \left\{ x \mid x \in \mathrm{R}^n;\ x^{LO} \le x \le x^{UP} \right\} \qquad \text{(RTSI-MINLP)}_k$$

$$y_l = Y_l,\ \forall l \in L;\ Y_1 \cup Y_2 \ldots \cup Y_L = Y = \{0,1\}^m$$

$$\varepsilon_k = \varepsilon_{k-1} - \Delta\varepsilon$$

It enables to identify profitable solutions with the maximal unburdening of the environment

Total Effects
RTSI-based Pareto Solutions, MINLP II

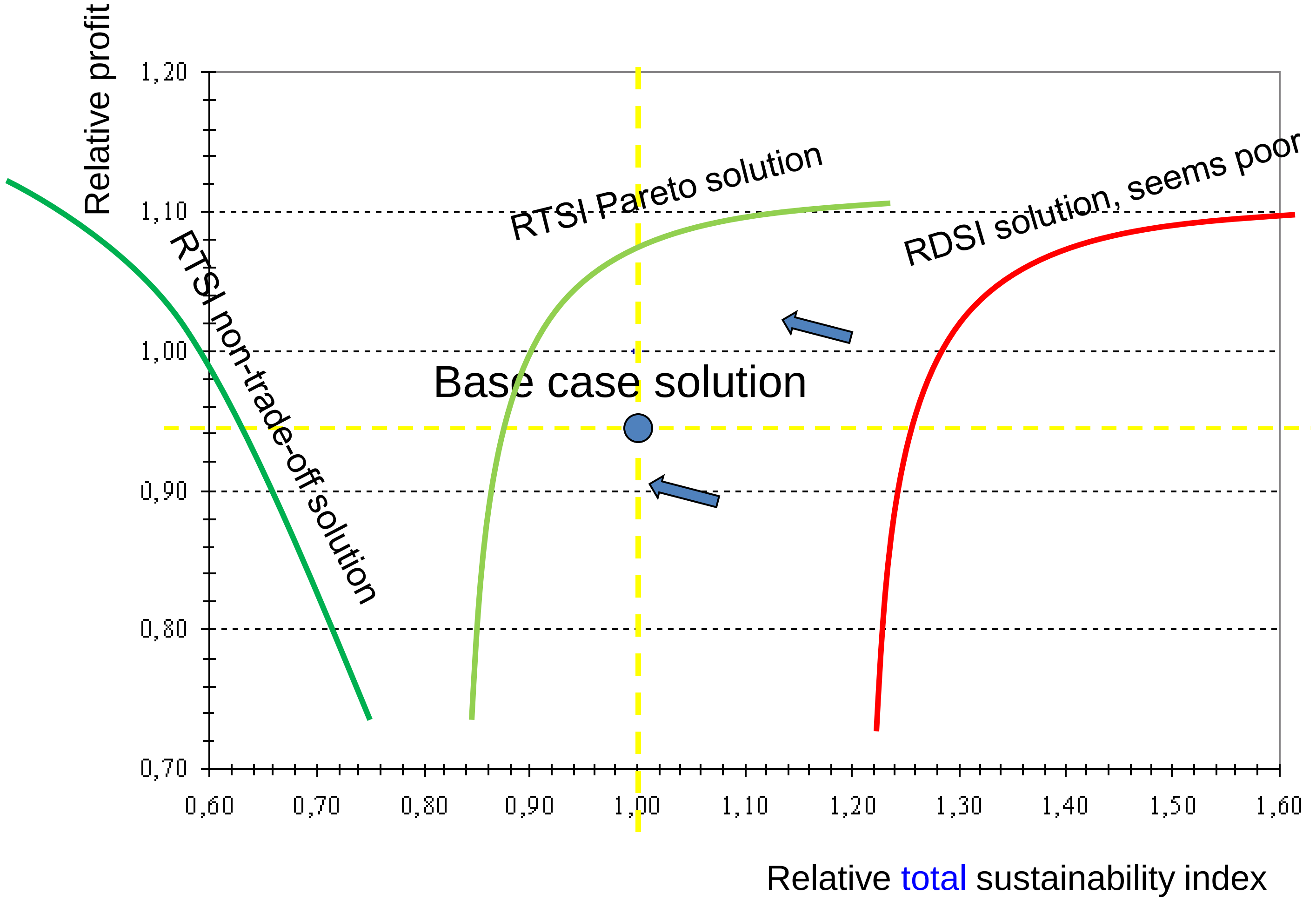


Fig. 32: RTSI Pareto or even non-trade-off solutions

5.2.2 Case Study: Bioethanol and RTSI

Main Motivation:

European Union targets are by 2020 to achieve at least

- a 20 % share of energy from renewable sources
- a 20 % improvement in energy efficiency
- reduction in greenhouse gas emissions
- a 10 % share of energy from renewable sources in transport

Main goal to reach or exceed 10 % of the need for gasoline in one European Country

Simultaneous integration of different technologies for converting starchy and lignocellulosic raw materials to bioethanol

Synthesis of Multi-Technologies Process

Variable raw materials input from the area of 50 000 ha and
Variable total production of ethanol

Optimization variables

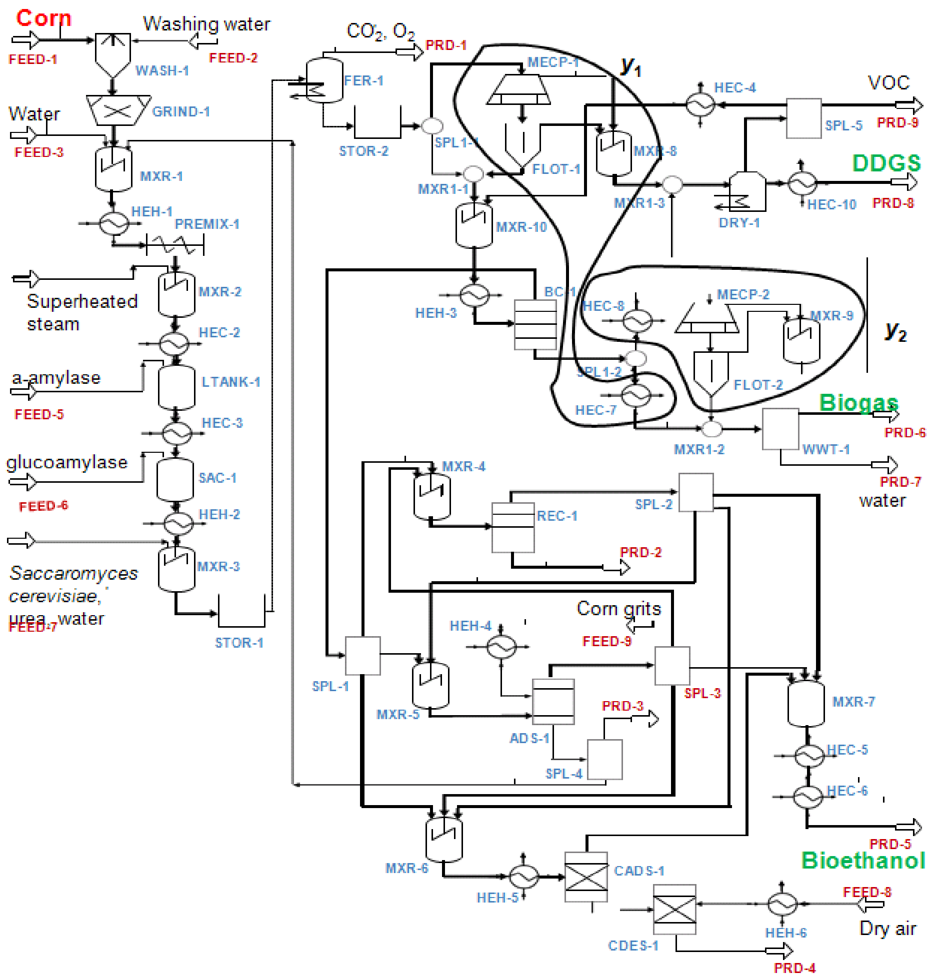
Footpint-based MINLP synthesis with:

- **MINLP-1:** Corn based ethanol production 2 kg/s (10 % share of bioenergy)
- **MINLP-2:** Energy and different food production
  (≤ 50 000 ha)

Bioethanol Process Synthesis Economic-based MINLP Step I

Karrupiah et al., 2008

Kravanja and Čuček, 2010

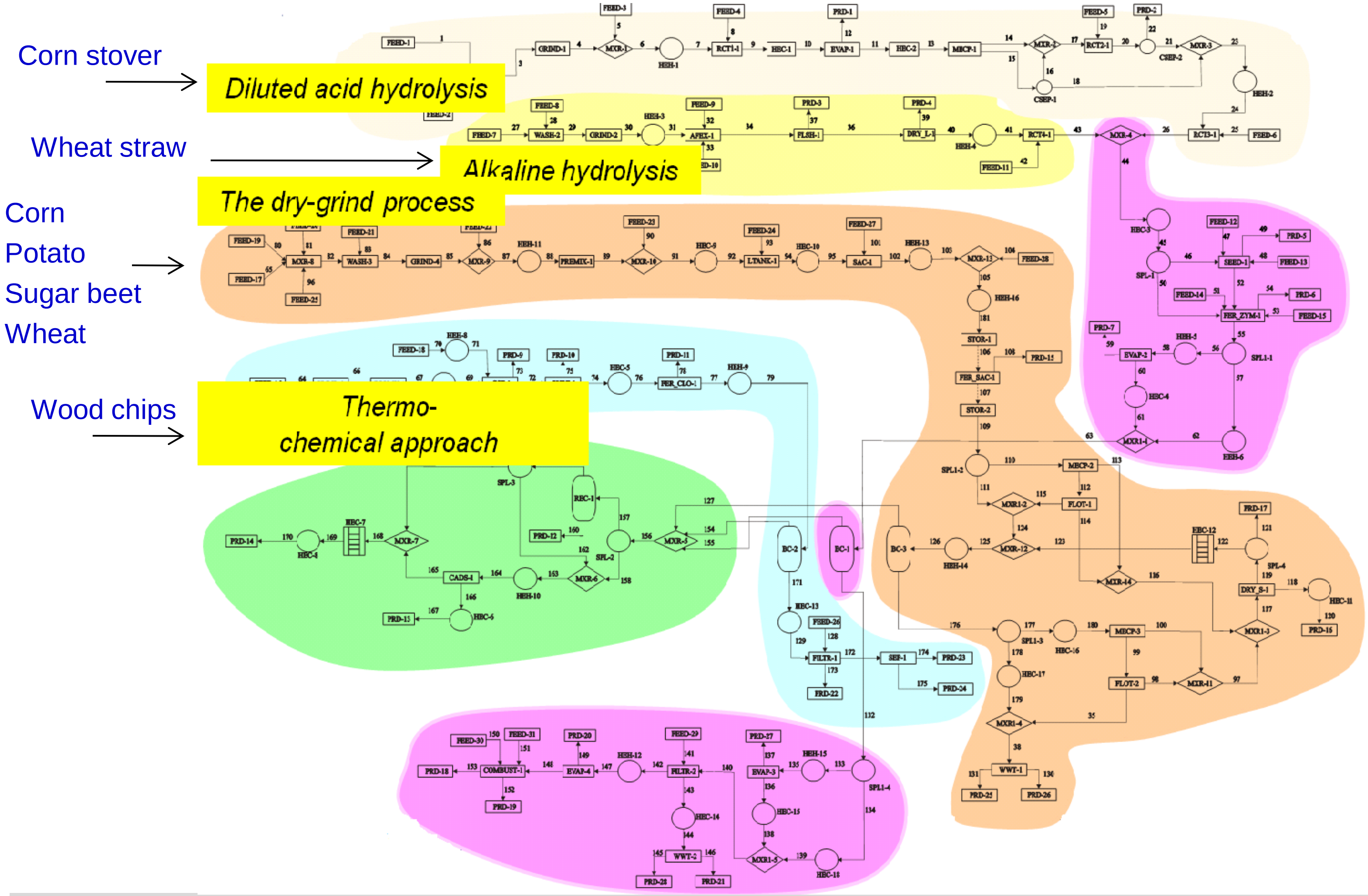


Solution:

P=22.786 M$/yr

Fig. 33: Corn-based process superstructure (1st generation)

Bioethanol Process Network Multiobjective Sustainable MINLP Step II



Corn stover

Diluted acid hydrolysis

Wheat straw

Alkaline hydrolysis

Corn
Potato
Sugar beet
Wheat

The dry-grind process

Wood chips

Thermo-chemical approach

Fig. 34: Superstructure, enlarged by sustainable alternatives (2nd generation)

Direct: SI-based Bioethanol Synthesis Multiobjective Sustainable MINLP Step II

Economic indicator:

$$RP = \frac{P}{P^0},\ where\ P^0 = 22.786\ M\$/yr$$

Relative direct sustainability index (RDSI):

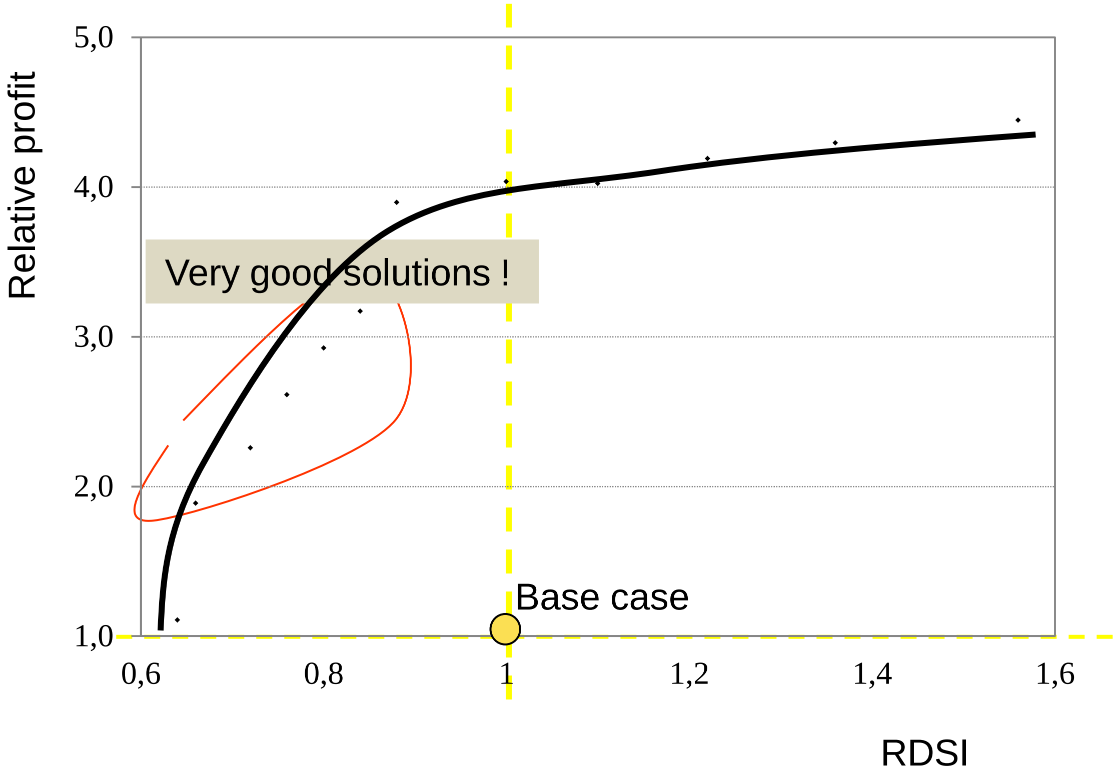
Intention is to obtain solutions with smaller CO2 equivalent emissions and to produce ethanol from raw materials, not part of the food chain. Weights:

- ⅓ CO2 emissions to the air
- ⅓ social indicator (food to energy)
- ⅓ all other indicators

$$\mathrm{RDSI} = \frac{1}{3}\cdot\frac{q_{m,ea}}{q^0_{m,ea}} + \frac{1}{3}\cdot\frac{q_{m,fe}}{q^0_{m,fe}} + \frac{1}{3}\cdot\frac{1}{9}\cdot\left(\frac{q_{m,su}}{q^0_{m,su}} + \frac{q_{m,fu}}{q^0_{m,fu}} + \frac{q_{m,pu}}{q^0_{m,pu}} + \frac{q_{m,wu}}{q^0_{m,wu}} + \frac{(A/q_m)_{land}}{(A/q^0_m)_{land}} + \frac{q_{m,fc}}{q^0_{m,fc}} + \frac{q_{m,eu}}{q^0_{m,eu}} + \frac{q_{m,es}}{q^0_{m,es}} + \frac{q_{m,ew}}{q^0_{m,ew}}\right)$$

Direct: SI-based Solution from Multiobjective MINLP Step II

Scalar parametric optimization:



Variable raw materials input from the area of 50 000 ha

Variable total production of ethanol

Fig. 35: “Pareto curve” for Bioethanol problem obtained by RDSI

Direct: SI-based Bioethanol Synthesis Solution: Energy and Food Production

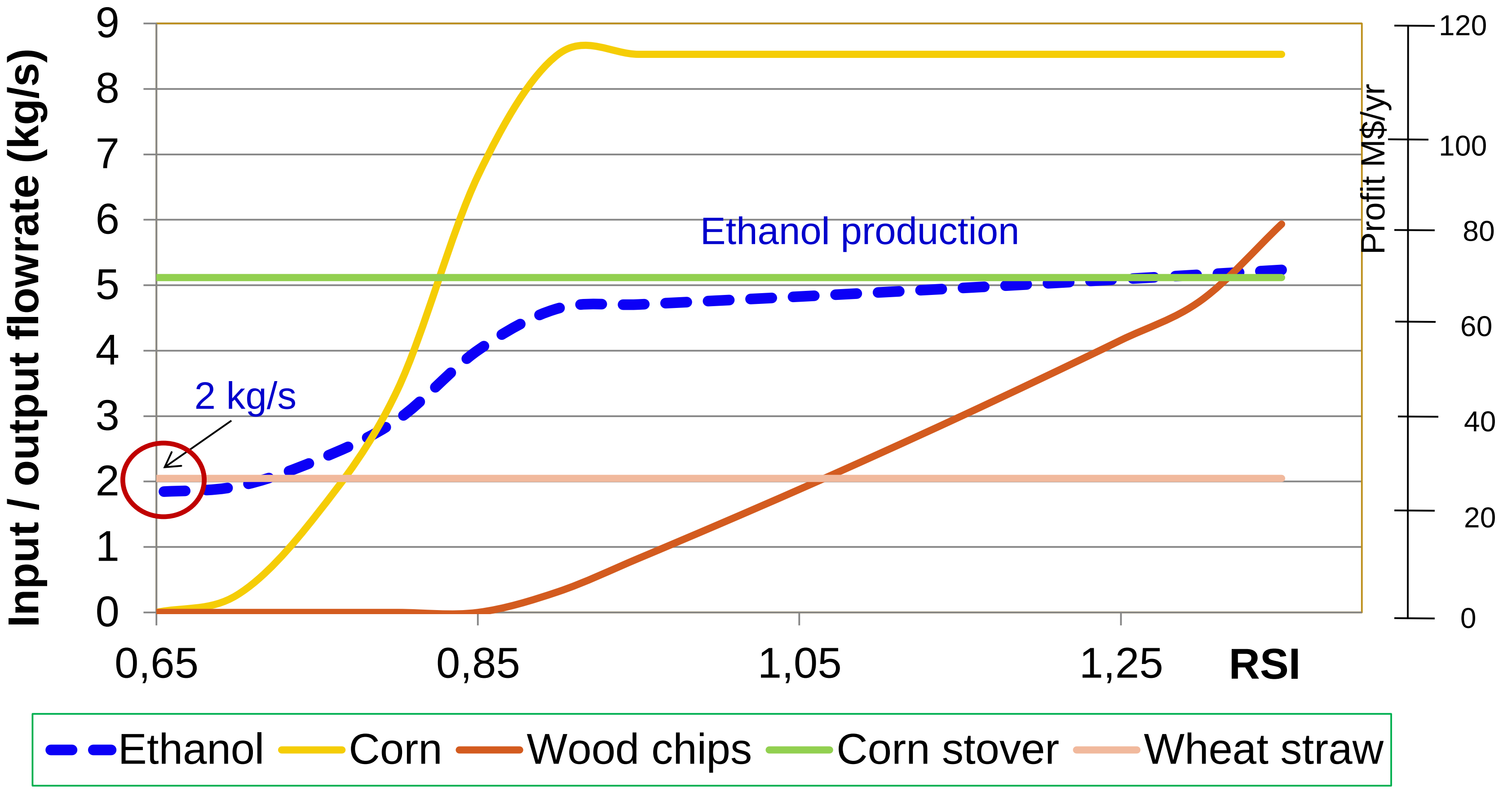


Fig. 36: Raw material and bioethanol production by RSI

Total SI-based Bioethanol Synthesis Multiobjective Sustainable MINLP Step II

Relative total sustainability index (RTSI)

Direct and Indirect CO2 equivalent emissions
Indirect effects due to products‘ substitution (gasoline by bioethanol)
The same weights as before:

- ⅓ CO2 emissions to the air
- ⅓ social indicator (food to energy)
- ⅓ all other indicators

$$\mathrm{RTSI} = \frac{1}{3}\cdot\left(\frac{q_{m,ea}}{q_{m,ea}^{0}} \boxed{- \frac{q_{m,ea}^{\mathrm{Ethanol}}}{q_{m,ea}^{\mathrm{Ethanol},0}}\cdot f_{\mathrm{Gasoline/Ethanol}}^{\mathrm{Sub}}}\right) + \frac{1}{3}\cdot\frac{q_{m,fe}}{q_{m,fe}^{0}} +$$

$$\frac{1}{3}\cdot\frac{1}{9}\cdot\left(\frac{q_{m,su}}{q_{m,su}^{0}} + \frac{q_{m,fu}}{q_{m,fu}^{0}} + \frac{q_{m,pu}}{q_{m,pu}^{0}} + \frac{q_{m,wu}}{q_{m,wu}^{0}} + \frac{(A/q_m)_{land}}{(A/q_m^{0})_{land}} + \frac{q_{m,fc}}{q_{m,fc}^{0}} + \frac{q_{m,eu}}{q_{m,eu}^{0}} + \frac{q_{m,es}}{q_{m,es}^{0}} + \frac{q_{m,ew}}{q_{m,ew}^{0}}\right)$$

Total SI-based Solution from Multiobjective MINLP Step II

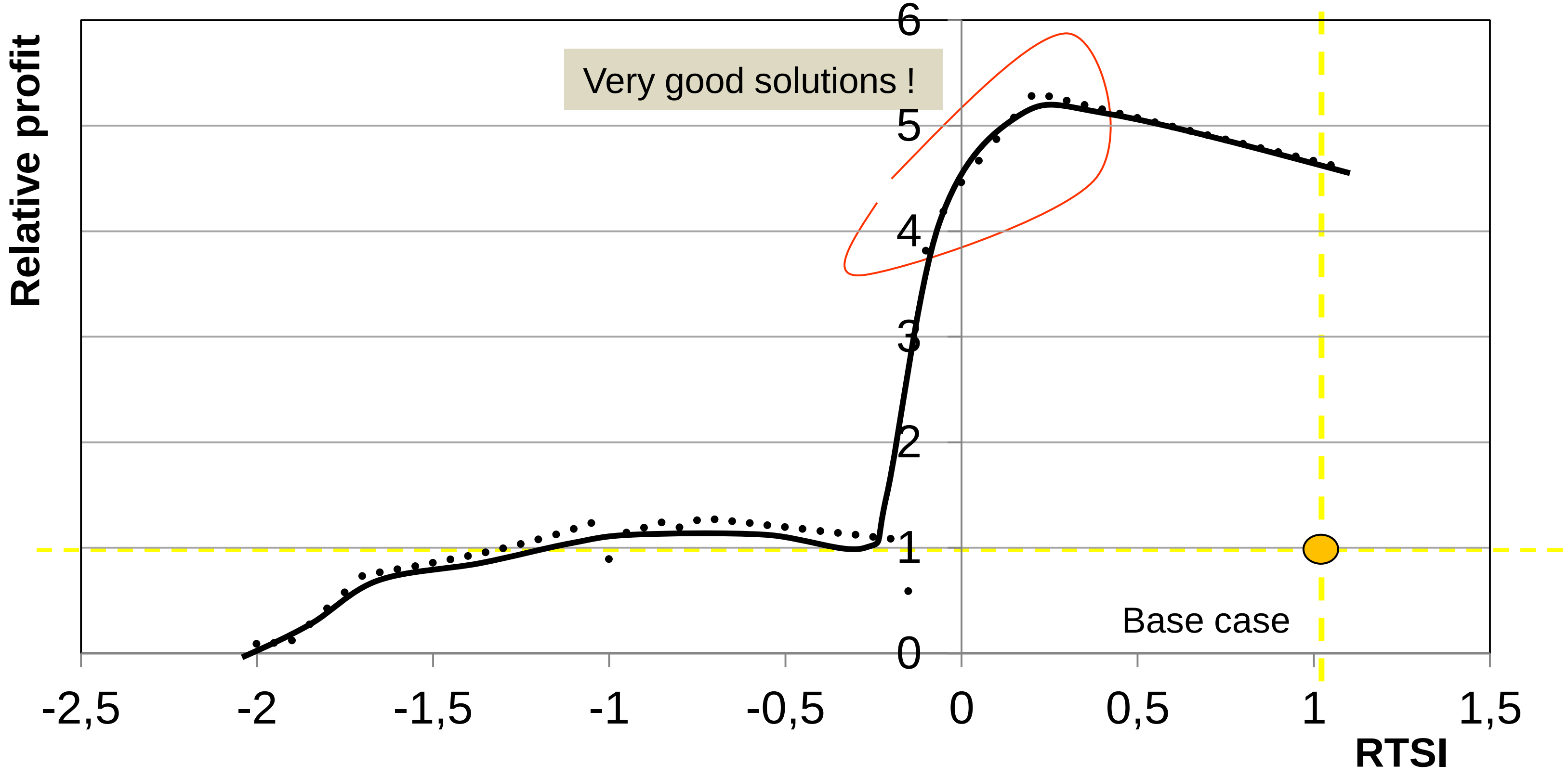


Fig. 37: “Pareto curve” for Bioethanol problem obtained by RTSI

5.2.3 Case Study: SI-based MINLP Synthesis of Biogas Process

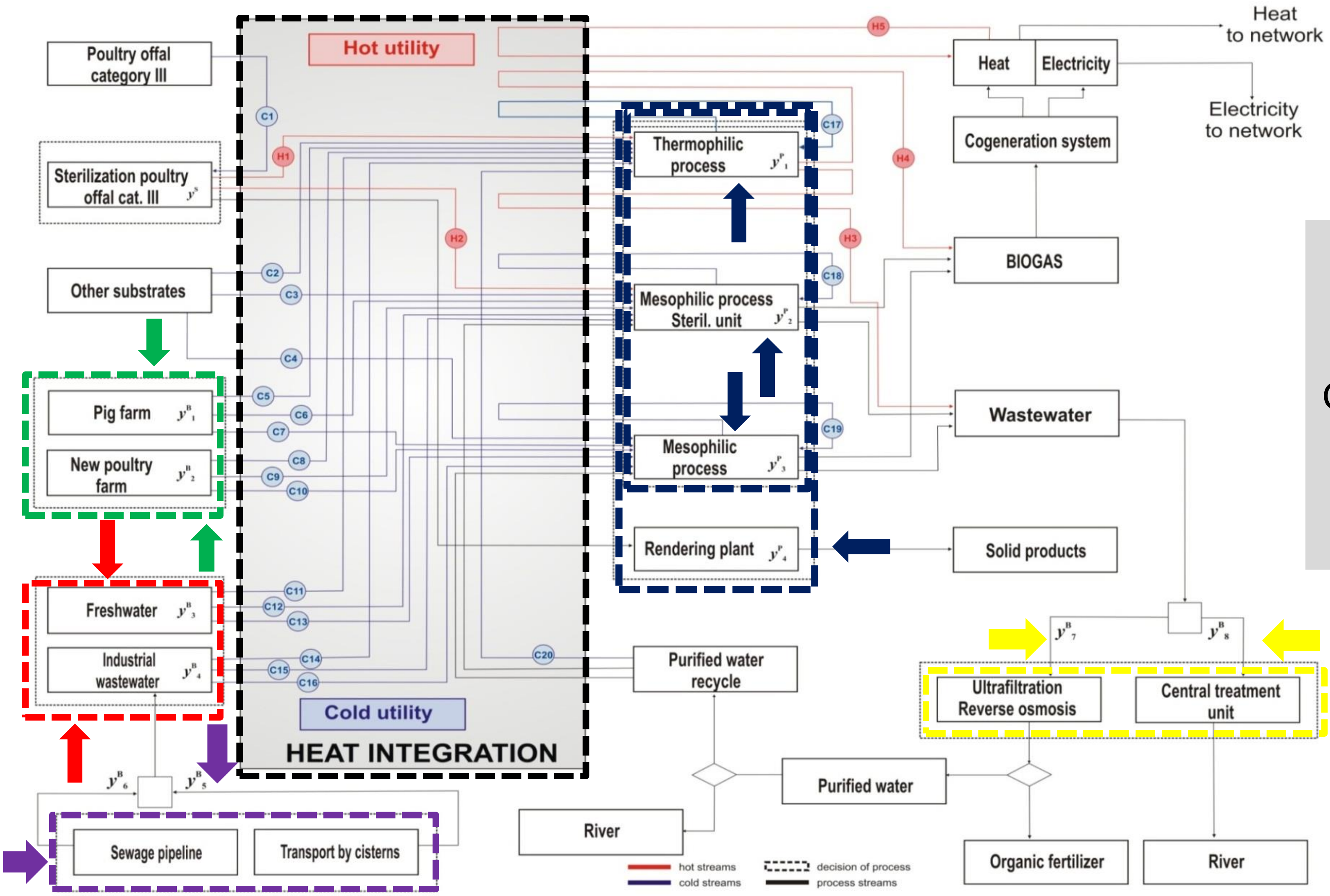


Fig. 39: Biogas from Organic and Animal Waste

study

Case Study: SI-based Synthesis MINLP Step II

Economic indicator: *Annual profit*

RSI index:

Intention to obtain solutions with smaller CO2 equivalent emissions

Weights:

- ½ CO2 emissions to the air
- ½ all other indicators

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

rϵR={carbon footprint (CF), agricultural land footprint (ALF), water consumption (WS), nitrogen footprint (NF)}

CF^0, ALF^0, WS^0, NF^0 taken from MINLP-I solution

LCA software package GaBi® (PE, LBP, 2011)

Ecoinvent database (Frischknecht et al., 2007).

Case Study: RSI-based Solution from Multiobjective MINLP Step II

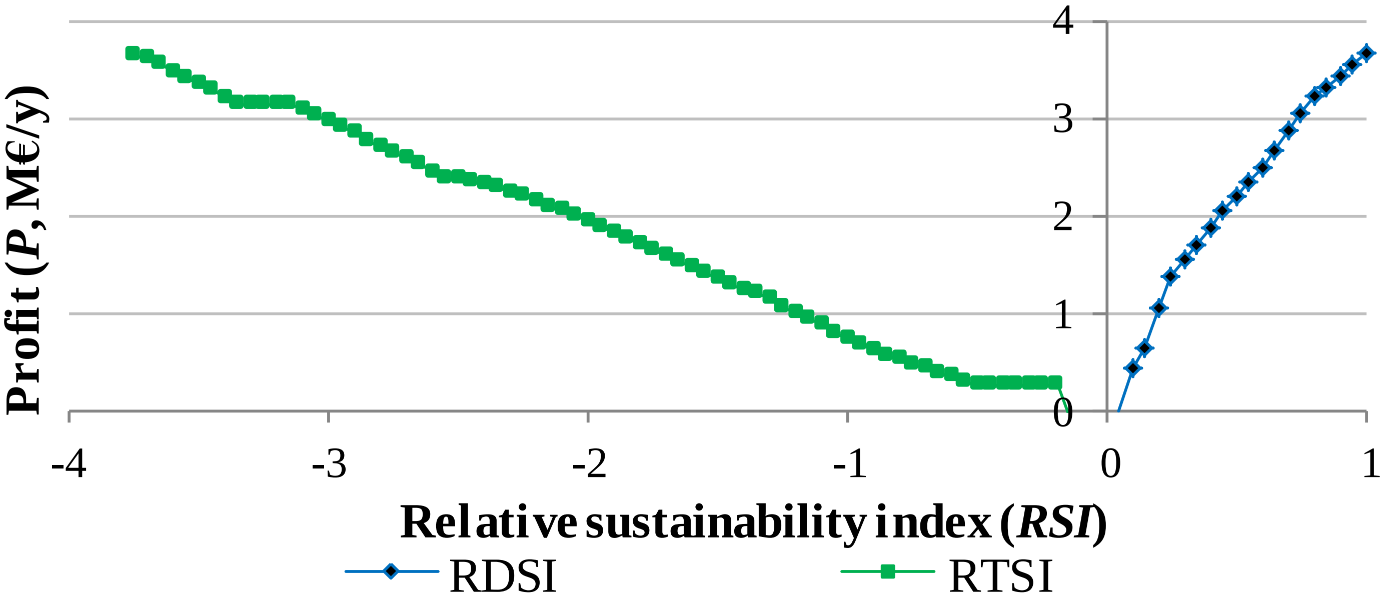


Fig. 40: A Pareto curve for RDSI and a set of non-trade-off solutions for RTSI

SI-based Synthesis

ADVANTAGES

- SI-based optimization suitable for:
  - Any number of footprints
  - Medium- and larger-sized problems

DRAWBACKS

- Subjective definition of weights

Drawbacks of RDSI:
- Wrong solutions - unsustainable

Drawbacks of RTSI:
- Cannot predict true trade-off solutions

- Incentives for Sustainable Development
- LCA-based Mathematical Programming for Sustainable System Synthesis
- Expanding Systems Boundaries
- Tools and Concepts Integration
- New Concept Considering Burdening and Unburdening Effects on Environment in Multiobjective Optimization:
    - Total Footprints,
    - Total Sustainability Index, and
    - Eco-Profit and Total Profit
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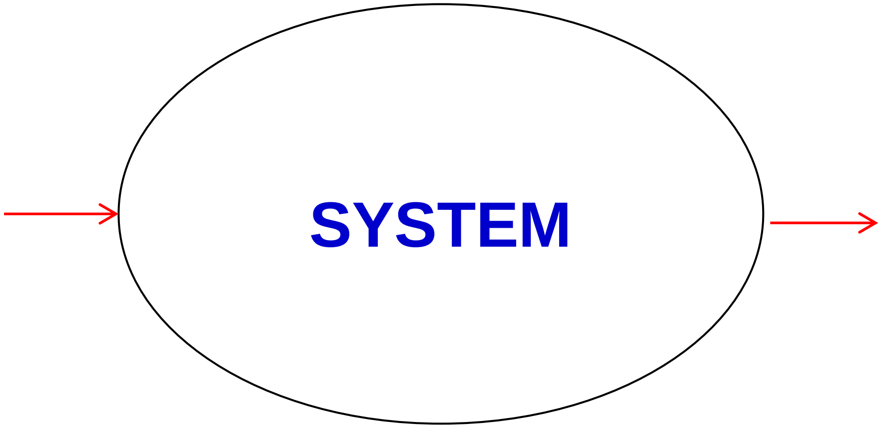
5.3.1 Direct Effects in Composite-Criterion: Net Profit

R – raw materials, which directly burden the environment due to:

- Extraction of resources,
- Recycling and
- Transportation



SYSTEM

P – *set of products, which directly burden the environment due to:*

- *Processing,*
- *Transportation,*
- *Use and*
- *Disposal*

Eco-cost (€/yr) :

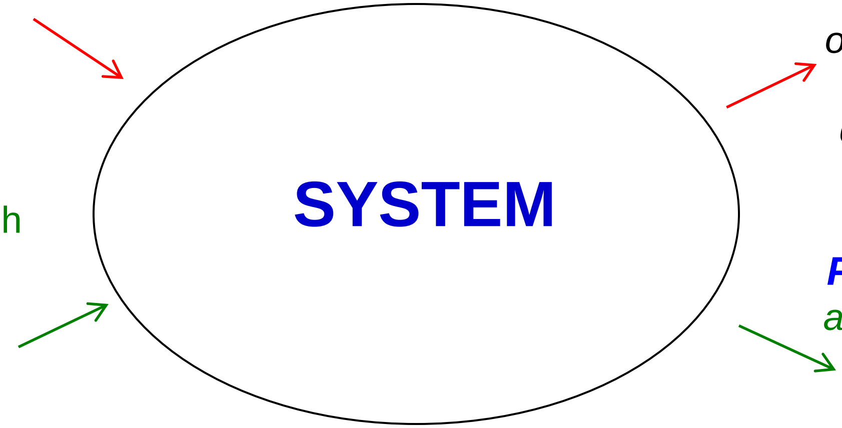
$$EC = \sum_{i \in R} q_{m_i}^{\mathrm{R}} \cdot c_i^{\mathrm{d,R}} + \sum_{k \in P} q_{m_k}^{\mathrm{P}} \cdot c_k^{\mathrm{d,P}}$$

Net profit (€/yr) = Economic profit - Eco-cost

$$NP = (R - E - D) - EC$$

Eco-cost coefficients: Delft University of Technology, <www.ecocostsvalue.com>

5.3.2 Total Effects in Composite-Criterion: Total Profit



R_B – raw materials, which only burden the environment if they are processed (direct effects)

R_{UNB} – raw materials, which mainly unburden or benefit the environment when they are used , e.g. utilization of waste (*direct +indirect effects*)

SYSTEM

P_B – *set of products, which only burden the environment related to processing, disposal, and transportation (direct effects)*

P_{UNB} – *set of products which alco unburden or benefit the environment (direct +indirect effects)*

Eco-profit(€/yr) = Eco-benefit - Eco-cost

Eco-benefit (€/yr): $$EB = \sum_{i \in R_{UNB}} q_{m_i}^{\mathrm{R_{UNB}}} \cdot c_i^{\mathrm{R_{UNB},t}} + \sum_{j \in P_{UNB}} q_{m_j}^{\mathrm{P_{UNB}}} \cdot f_j^{\mathrm{S/P_{UNB}}} \cdot c_j^{\mathrm{S,t}}$$

Eco-cost (€/yr) : $$EC = \sum_{i \in R_{\mathrm{B}}} q_{m_i}^{\mathrm{R_B}} \cdot c_i^{\mathrm{d,R_B}} + \sum_{j \in P_{\mathrm{B}}} q_{m_j}^{\mathrm{P_B}} \cdot c_j^{\mathrm{d,P_B}} + \sum_{k \in R_{\mathrm{UNB}}} q_{m_k}^{\mathrm{R_{UNB}}} \cdot c_k^{\mathrm{d,R_{UNB}}} + \sum_{l \in P_{\mathrm{UNB}}} q_{m_l}^{\mathrm{P_{UNB}}} \cdot c_l^{\mathrm{d,P_{UNB}}}$$

Total profit (€/yr) = Economic profit + Eco-profit

$$TP = (R - E - D) + (EB - EC)$$

Čuček, Drobež, Pahor, Kravanja, 2012

Total Effects
Total Profit-based Synthesis

Čuček, R. Drobež, B. Pahor, Z. Kravanja, CCE, 2012

$$\max TP = P(y,x) + EcoP(y,x)$$

$$\text{s.t.} \quad \left.\begin{aligned} h_l(x, y_{ls}) &= 0 \\ g_l(x, y_{ls}) &\le 0 \end{aligned}\right\} \quad \forall l \in L, s \in S$$

$$x \in X = \left\{ x \mid x \in \mathrm{R}^n;\; x^{LO} \le x \le x^{UP} \right\} \qquad \text{(TP-MINLP)}$$

$$y_l = Y_l,\; \forall l \in L;\; Y_1 \cup Y_2 \ldots \cup Y_L = Y = \{0,1\}^m$$

Multi-objective problem converted into sinle-objective

5.3.3 Biogas Process Case Study Reconsidered: Total Profit-based MINLP

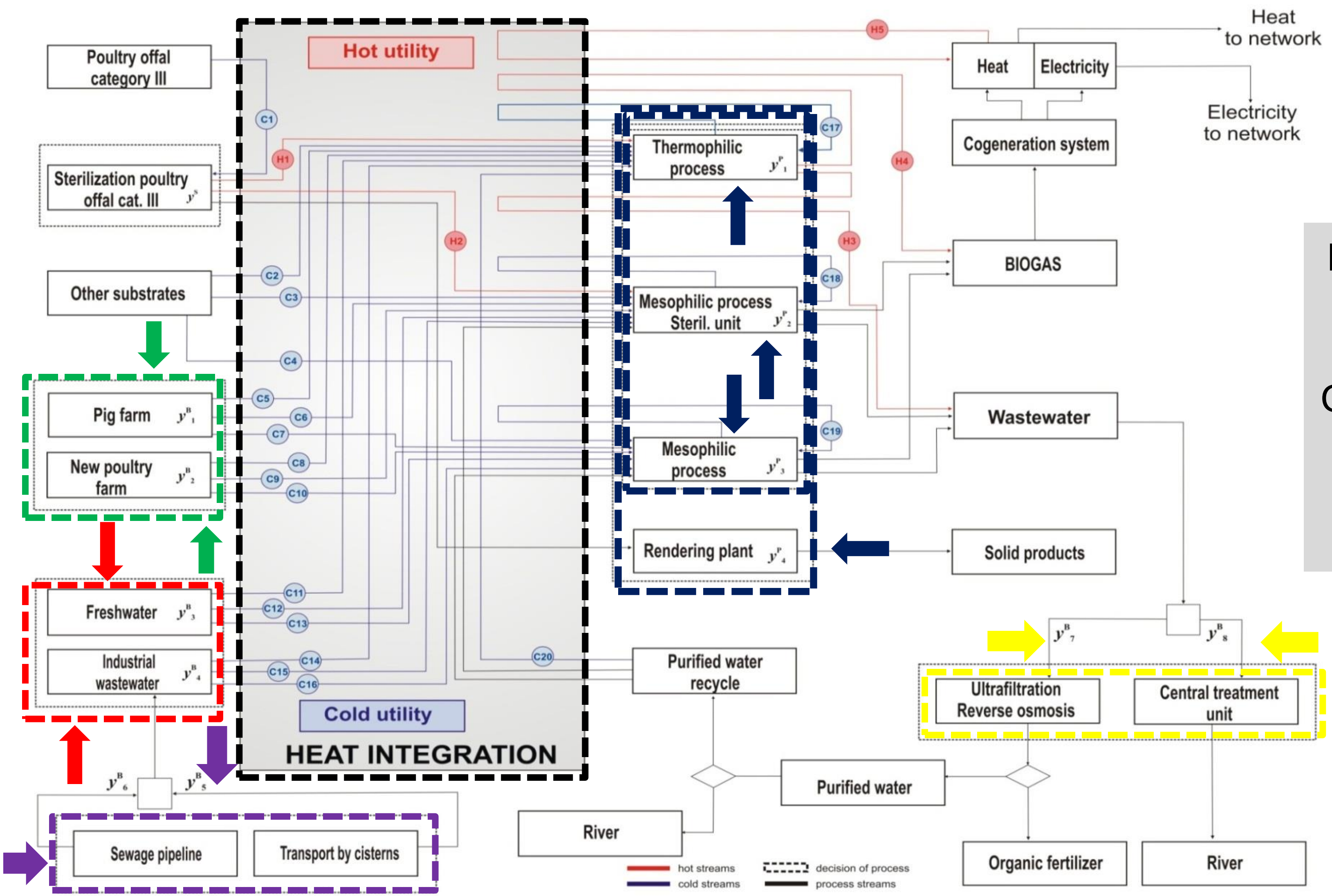


Fig. 41: Biogas from Organic and Animal Waste

study

Total Profit

Direct Effects: Economical and Net Profit Optimization

Table 2: Different optimization schemes with Eco-cost for Biogas problem

	Maximized Economic profit (*P*)	**Maximized Net profit (*NP*)**
Economic profit (M€/y)	3.308	**0**
Eco-cost (M€/y)	5.301	**0**
Net profit (M€/y)	-1.992	**0**
Income (M€/y)	7.546	**0**
Depreciation (M€/y)	2.943	**0**
Investment (M€)	20.727	**0**
Operating costs (M€/y)	4.238	**0**
Biogas production (m^3/d)	43,281	**0**
The amount of used wastes (t/y)	122,861	**0**

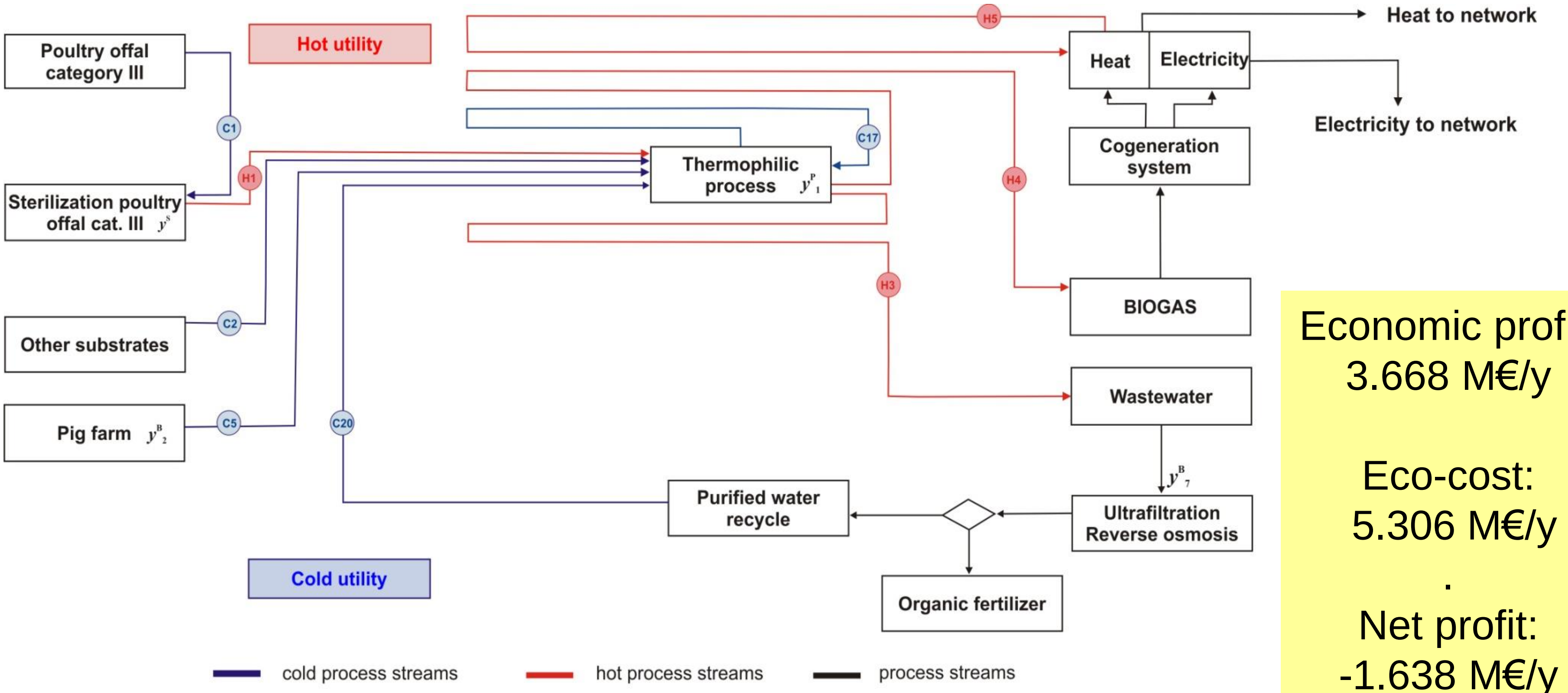
Total Profit

Direct Effects: Economical and Net Profit Optimization

Čuček, Drobež, Pahor, Kravanja, CCE, 2012

Kravanja, Čuček, APEN, 2013

Maximization of the **economic profit**



Economic profit:
3.668 M€/y

Eco-cost:
5.306 M€/y
.
Net profit:
-1.638 M€/y

Fig. 42: Optimal Biogas production flowsheet

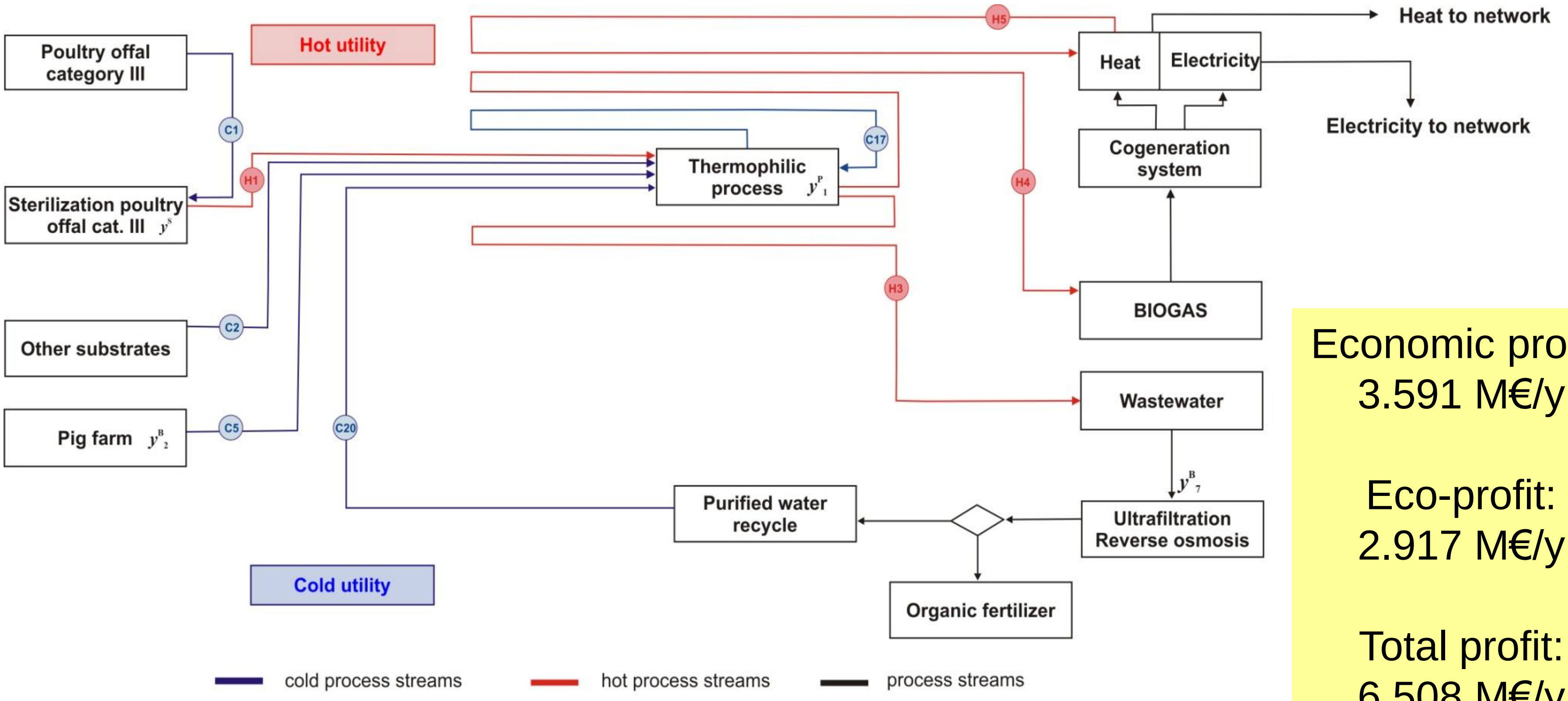
Total Effects: Total Profit Optimization

Table 3: Different optimization schemes with Economic and Total profit optimization

	Maximized Economic profit (*P*)	**Maximized Total profit (*TP*)**	Difference *TP-P*
Economic profit (M€/y)	3.668	**3.591**	-0.077
Eco-profit (M€/y)	2.661	**2.917**	+0.256
Total profit (M€/y)	6.329	**6.508**	+0.179
Income (M€/y)	7.354	**7.249**	
Depreciation (M€/y)	2.943	**2.925**	
Investment (M€)	20.727	**20.600**	
Operating costs (M€/y)	3.686	**3.658**	
Biogas production (m^3/d)	43,281	**42,623**	
The amount of used wastes (t/y)	122,861	**121,180**	

Total Effects: Eco-profit and Total Profit Optimization

Maximization of the **total profit**



Economic profit:
3.591 M€/y

Eco-profit:
2.917 M€/y

Total profit:
6.508 M€/y

Fig. 43: Optimal Biogas production flowsheet

Total Profit-based Synthesis

ADVANTAGES

- Direct solution procedure with composite objective
  - Very large-sized problems can be solved

5.3.4 Continental Example – EU Supply Network for the Production of Biofuels

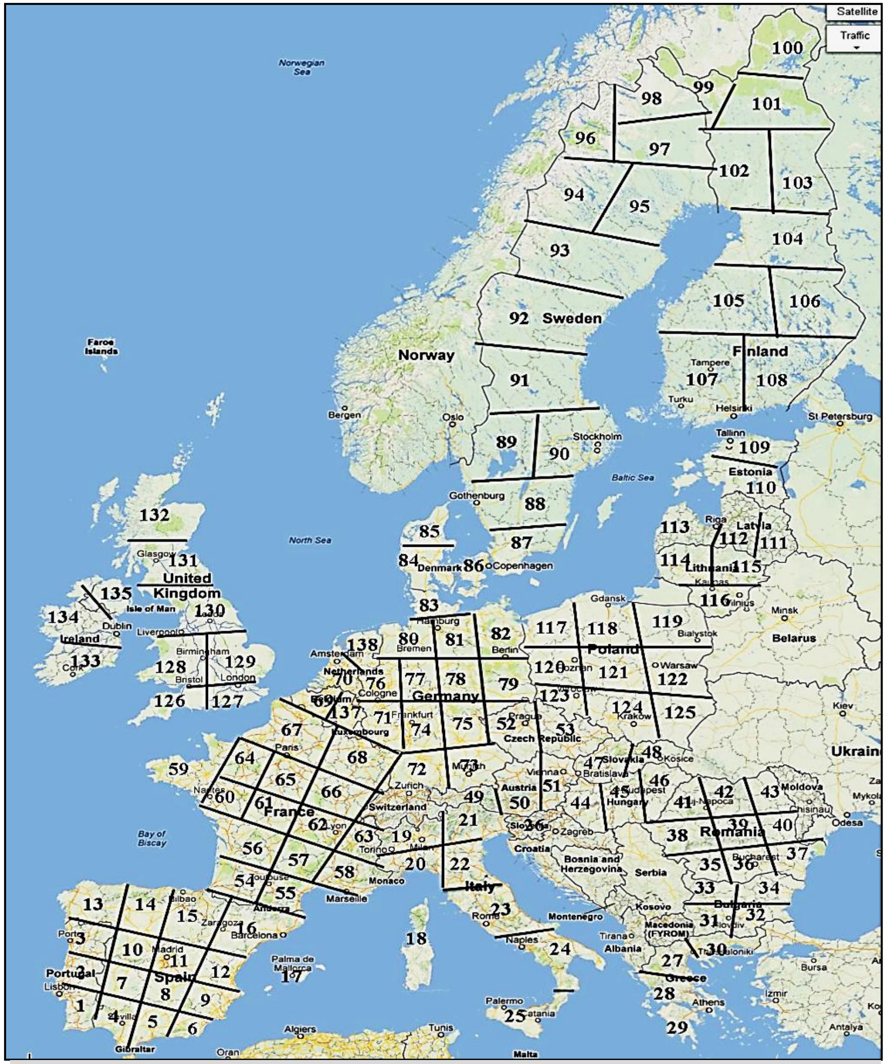


Fig. 45: Regional plan with 136 zones

Čuček, Martin, Grossmann, Kravanja, ICOSSE 2013, ESCAPE 24, 2014

Area for food and biofuels: ≤10 % area,
Demand: ≥ 100 % food, ≥ 10 % biofuels
Raw materials: 1st, 2nd, and 3rd generation
Technologies:
- Biochemical conversion
- Gasification and syngas fermentation and catalytic synthesis
- FT diesel and green gasoline
- Biodiesel from oils with methanol...

Products: Ethanol, Biodiesel, Hydrogen, Green gasoline, FT-diesel...

GAMS 23.6, GUROBI 4.0
Server with 244 GB of RAM

1,150,000 single equations
24,220,000 single variables
27,900 discrete variables

Redistribution of Gasoline production: Profit vs. CO_2-based Total Profit

0.135 EUR/kg CO_2 eq, www.ecocostvalue.com

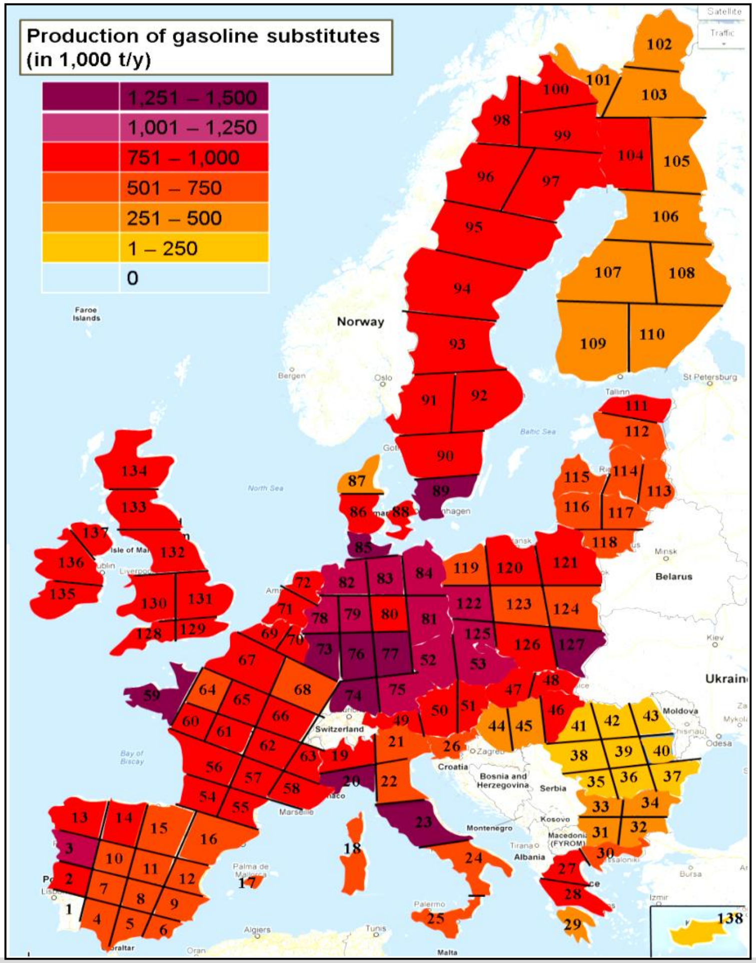


Fig. 46: Profit 134,457 M$/y,
67.8 % substitution

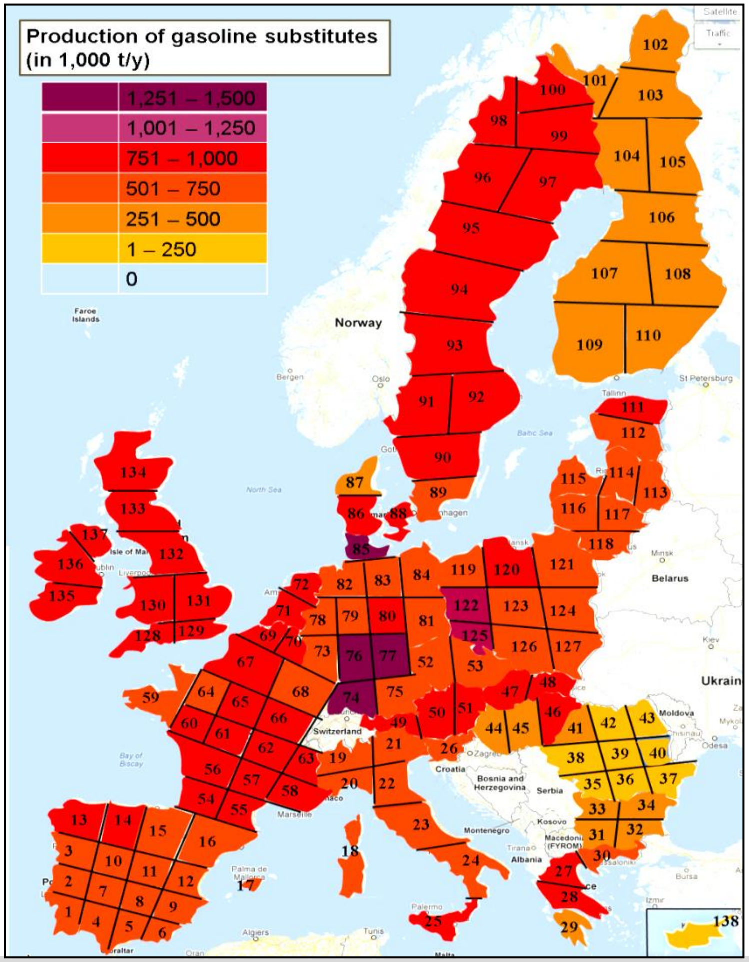


Fig. 47: Total Profit 155,655 M$/y,
63.9 % substitution

Total Profit

Conclusion

- The role of holistic approach was highlighted for sustainable systems synthesis.
- When considering only direct (burdening) effects on environment, incomplete and even wrong solutions can be obtained.
- Indirect (unburdening) effects caused by products‘ substitution should also be considered in MOO.
- New perception:
  - Better searching solutions by maximizing the difference between unburdening and burdening effects than just minimizing burdening effects.
  - Unburdening alternatives will thus have higher priority than those having just smaller burdening effects.

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ESCAPE 2016, Portorož, Slovenia

PORTOROŽ, COAST & KARST REGION

The poetically named Portorož, or Port of Roses, is best described by the words: sea, wind, salt, Mediterranean aromas, palm trees, roses and evergreens, relaxation, fun and friendliness. Portorož has been a tourist destination since as far back as the 13th century. This reputation persists even today.

Every kilometre of the Slovene coast is a new surprise. Here is a natural reserve of rich marl and sandstone and the unique, eighty-metre Strunjan cliff, the highest flysch wall on the Adriatic coast. Not far from the coast, the beauties of Slovenian Istria with its picturesque villages await you. Amongst them, for example, is Hrastovlje with its Holy Trinity church decorated with narrative late Gothic frescoes including a magnificently preserved Danse Macabre.

Inland from the Slovenian coast is the Karst region. In the cellars of the stone houses excellent wines are poured and sold, and in the attics excellent pršut is cured in the bora wind. This gourmet paradise is also a heaven for lovers of the beauties of the karst underworld. The Škocjan Caves, which are on UNESCO's list of natural and cultural world heritage sites. However there is another gem one should visit— The Postojna Cave. It is the best-known cave in the world and one of the world's largest karst monuments.

And this is far from being the last of the attractions of Slovenia's karst region. Perhaps you don't know that the noble Lipizzaner horses (of the Vienna Riding school fame) originate in Slovenia. Lipica, where the stud farm was established in 1580, is today a popular tourist centre.

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