

MULTICRITERIA ASSESSMENT OF SHORT LIFE-CYCLE MATERIALS WITHIN THE CONTEXT OF SUSTAINABLE DEVELOPMENT AND ENERGY EFFICIENCY.

Abstract: This work will explore the creation of a methodology for a multidisciplinary problem in nature dealing then with Multicriteria decision making aid. The problem considers the role of energy use in sustainable development and the potential sources to increase energy efficiency during life cycle use of some materials used in a day to day basis. A set of criteria to make decisions to choose alternative materials are among other: Exergy loss, Green House Gases emissions, real energy flows and material balances needed to the chain of manufacturing processes in the productions and value added. Nevertheless, thinking in alternative materials to substitute the actual ones, it is necessary to look forward. That's why we will also use some other tools in order of complain a set of alternative materials for a long term use.

Introduction.

Scientific and technological development enables to provide a wide variety of goods and services in order to satisfy our day to day needs; nevertheless they also put in risk the quality and longer-term viability of the biosphere as a result of unwanted, 'second order' effects [1]. These effects are those related to pollution, as mainly global warming, acid rain, water and soil contamination, etc.

The international community has decided the concept of 'sustainable development', by Bründlandt report that considers sustainable development as: the development that meets the human needs of the present without compromising the ability of future generations to meet their own needs [2], it continues to be evident that sustainability is a multidisciplinary topic including challenges for technology, based on the efficient use of energy. A lot of parameters and criteria are essential for long-term global sustainability.

Our thesis concerns to different materials or ways to use them getting longer use life cycle, saving energy and avoiding pollution; we strongly believe that using technology, sustainability without wasting nonrenewable resources and energy, is possible.

Based on the definition of sustainable development and the growing interest in the development of policies focused on the generation of environmentally appropriate products and services, the use of life-cycle analysis has required the incorporation of criteria which make more robust this concept. Within the framework of sustainable development, energy efficiency has been linked successfully with the concept of exergy, incorporating the Exergy life cycle Analysis (Cornelissen, R. L., 1997), where exergy consumption (destruction) is considered an important criterion to define, among other criteria, the minimization of the irreversibility of exergy deposits of natural resources at levels which have minimal environmental impacts to ensure life-support systems to the following future generations. With the exergetic life cycle analysis, it is possible to measure quantitatively the depletion of non-renewable resources and then, to avoid them. The exergy and life cycle analysis can then be incorporated as a performance criterion to compare diverse end-use daily materials.

On the other hand, the majority of organic chemical compounds and polymers are still derived from fossil based feedstocks, i.e. oil and gas. Non-energy applications of them account for around 9% of all fossil hydrocarbons (oil, gas, coal) use and 16% for oil products (Shen, L & Patel, M). Global petrochemical production of chemicals and polymers is around 335 million tonnes. Primary output comes from a reduced number of key building blocks as methanol, ethylene, propylene, butadiene, benzene, toluene and xylene. These building blocks are converted to polymers and plastics and also to a an important number of specialty chemicals with specific functions.

At this stage is necessary to note that from technical point of view almost all industrial materials made from fossil resources could be substituted by their bio-based counterparts.

The Meaning energy efficiency.

The reduction of the “energy consumption” is, from the ecological view, the priority goal. The reduction of carbon-dioxide emissions is again it only a partial goal.

From a company view, energy-cost reduction is the main goal for investment in efficient equipment. Thus efficiency evaluation takes place according to different criteria. From technical view, the primary energy input used for a useful output has to be minimized.

It is common to define a total coefficient for efficiency by adding power and heat, without taking into account that both have for the same quantity of energy given for example in MWh different quality ratings. Energy-technical optimizations must therefore have always considered the content of exergy. Electric current contains energy with the exergy factor 1 of unity, while heat has a lower exergetic potential, which, dependent on the temperature in accordance with the Carnot factor. 1 MWh process steam may be equated in no case with 1 MWh room heat and not at all with 1 MWh electric current.

To select which material (including the actual ones) is better and to choose the outranking substitution alternatives, Multicriteria methods [3] can be used, considering several criteria such as: Exergy efficiency and irreversibility; nonrenewable resources used over their life cycle; profit and value added and GHG emissions created among manufacturing processes, are suitable criteria to remedy the use of materials waste.

In using the above concepts and methods to apply to some present materials used, it is presented in Figure 1, all the associated concepts that can be viewed integrally when developing this work.

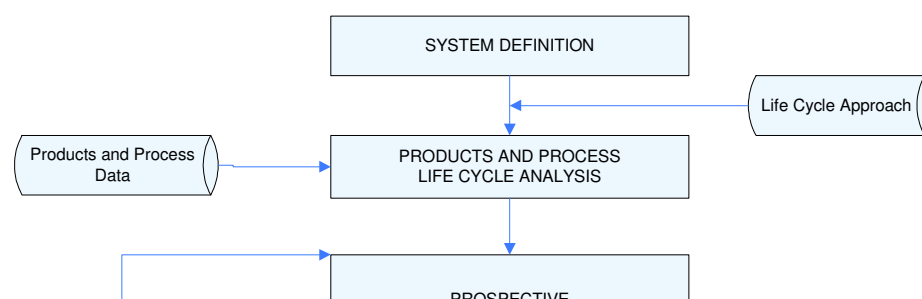


Figure 1. General description of the methodology.

In Figure 2, it is shown the relationship between sustainable development and efficient use of energy as we understand the problem.

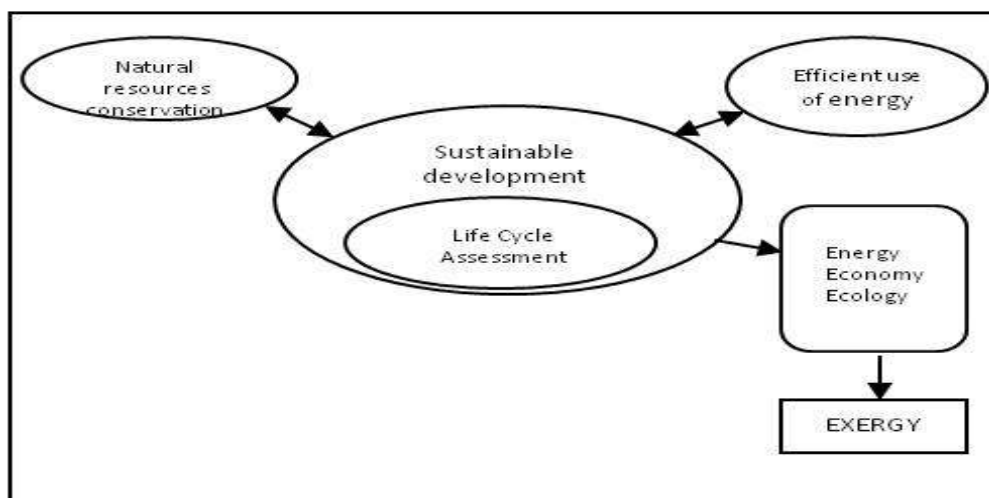


Figure 2. Relationship between sustainable development and efficient use of energy.

Objectives of this work

The objectives of the work are to develop a multicriteria decision aid assessment for the evaluation and selection of sustainable solutions for the production of daily-used materials such as for instance plastic bags, cups and bottles and to help decision-makers to achieve better energy efficiency and natural resources

conservation. Current practices are not efficient on the energy efficiency point of view and generate global pollution and waste problems within their complete life-cycle including production, use and disposal.

In order to achieve sustainable development multiple objectives have to be taken into account including economic factors as well as environmental or social impacts. This problem is thus very well suited to a multicriteria approach: multicriteria models and decision aid methods are designed to handle evaluation or decision problems involving several possible decisions that are evaluated on multiple and often conflicting evaluation criteria.

We propose to develop a methodology to evaluate and compare alternative solutions for the production of daily-use materials based on their life-cycle analysis, and to apply it to a Mexican case study. In a first time evaluation criteria will be defined in the context of sustainable development. Considering that we want to get an analysis in the long term, we will need prospective techniques to create scenarios for new materials and then, use systems dynamics for long term analysis. Preferences will be modeled using the PROMETHEE multicriteria decision aid methods and conclusions will be drawn from the subsequent analysis.

Then the project aims to use the methodology developed by *Escobar-Toledo et al, (2011)*, to analyze alternative technologies related to the production of end use materials (used in everyday life). The offer as the long term demand of the selected materials will both be analyzed in order to optimize the efficient use of energy, the conservation of resources and the ecological effects of materials in the different stages of their life cycles including the chain of intermediate products and associated processes.

The life cycle study of those kinds of products in their production chains will be applied since the raw material until they are disposed. In particular, we want to use the Exergy analysis as a quantitative tool to optimize Thermodynamics life cycle of plastics, including the possibility of recycling them when they are discarded or that are susceptible to produce energy through various other processes.

Partial objectives.

I. Identify the technological routes of production of those materials of end use and their respective substitutes that come from renewable or non-renewable natural resources that use energy efficiently and sustainably and serve as a means to optimize the processes of production (*Azapagic, a., 1999*)

II. Analyze the processes of selected materials that intensively use energy starting from basic commodities, intermediate and finals concerning the chain of production of materials of daily use materials will be analyzed, coming mainly from chemical and petrochemical industries (*Escobar Toledo EC, C. GarcíaAranda, B. Mareschal, 2010*), but not only.

III. Use of exergy analysis to quantitatively measure energy efficiency and life cycle of process and technology of product (*Rothstein, e., Stephanopoulos, g. 1999*).

IV. Identify technology transitions that allow the manufacture of basic, intermediate and final products using mainly natural renewable resources and alternative sources of energy in an efficient manner, taking into account the dynamics of the system studied in the long term. Discovering technological transitions as a high impact criterion to evaluate processes, sets an advantage in decision-making process and the consequently in planning, implementation and evaluation strategies for technological development (*Escobar-Toledo, C. Garcia A,2008*). See Figures 3 and 4.

Materials which will be used to manufacture end-use stuffs, will focus the optimization of existing processes or recycling after disposal, in order to obtain the "price or energy recovery bonus" considered as additional added value to the scientific point of view, the contributions of technology transitions and other disciplines could find a niche of opportunity for the development of knowledge in multidisciplinary fields.

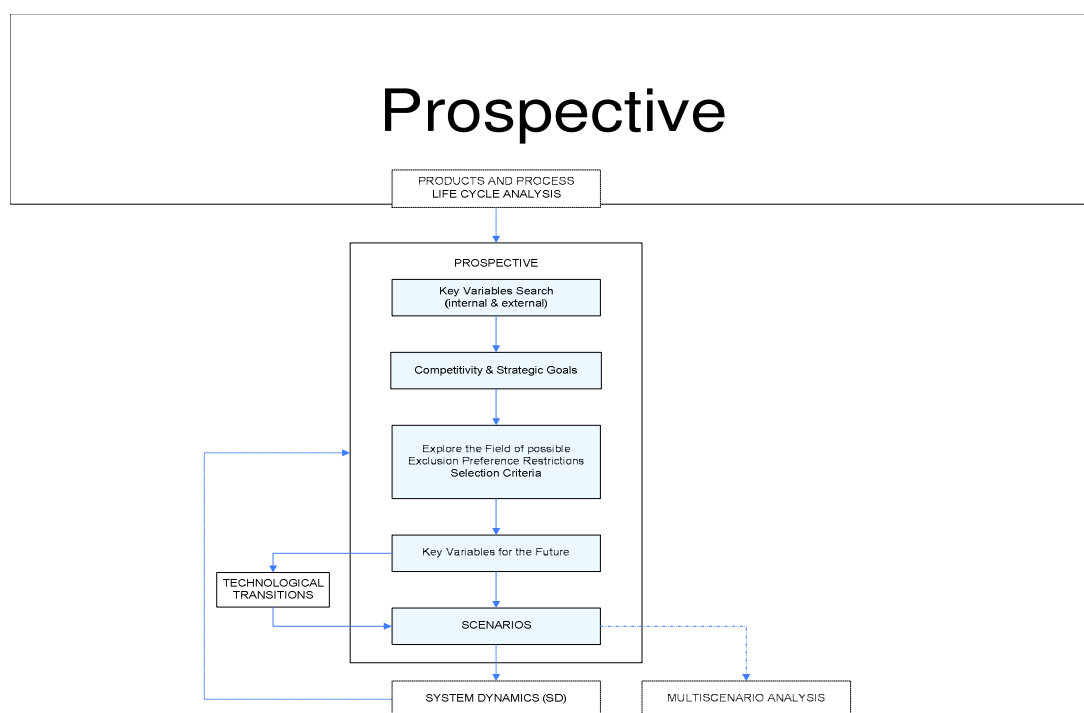


Figure 3: Prospective to be used in the methodology assessment.

System Dynamics

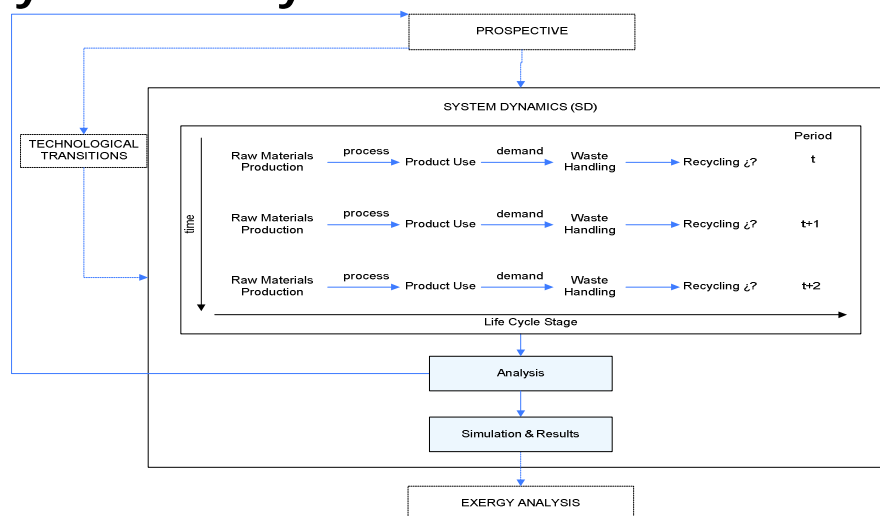


Figure 4: The role of Systems Dynamics in the project

V. Aid to final decision making, considering that there are various criteria to consider selecting and ranking technologies in the long term. See Figure 5.



Multicriteria Analysis

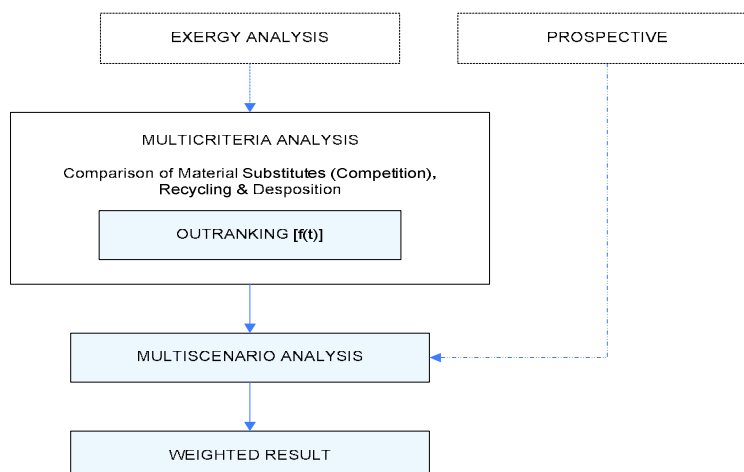


Figure 5. Representation of Multicriteria Analysis.

On the other hand, the emerging need for societal transitions raises the need for a better understanding of the dynamic nature of large scale societal systems, and therefore the development of an analytical approach for drawing dynamic conclusions based on system's dynamic mechanisms, feedback relationships and interacting components.

Another objective of this study could be to explore the degree to which System Dynamics as an approach enhances the process of understanding transition dynamics in sociotechnical systems. In other words, it is aimed to reveal the type of insights that can be developed about such systems and their dynamic behavior using the approach, as well as the shortcomings of the approach in this challenging task. In order to do so, a modeling study aiming to understand the underlying mechanisms of the waste management transition in the Netherlands is conducted.

The severity of the problems experienced in the socio-technical systems, and the rising concerns about the sustainability of the current functioning and the structure of the large-scale societal systems requires understanding how to change such systems.

Given the interconnection of social and physical/technological components in such systems, these processes of change are complex because these are long-term structural change processes spreading over several aspects of the societal system, such as culture, technology, institutions and infrastructure, and are referred to as *transitions* (Rotmans et al. 2001; Rotmans 2005).

These aspects of the transition processes are already discussed in literature (as for example, Loorbach 2007).

This difficulty raises the need for a better understanding of the dynamic nature of such systems. The dynamic complexity of the transition processes that makes them hard to comprehend arises mainly from the way the elements of the societal systems are arranged and the way they interact. These feedbacks may come from the technical, social and environmental domains, and some of these feedbacks are slow, whereas others are fast.

Methodology

The project will be organized in the following eight phases:

- 1) Problem definition

In this preliminary step, the problematic will be stated more precisely and a state-of-the-art review will be performed. The different stakeholders will also be identified in order to enable a multi-actor analysis.

2) Case study definition

The types of materials analyzed in the Mexican case study will be determined according to the general objectives and to data availability.

The alternative solutions for each type of materials will also have to be defined.

3) Criteria definition

The selection of the criteria that will be entered in the decision aid model is an important step. It will be performed based on the results of step 1. There are some definitions about criteria as: (1) Minimize the irreversibility in the production chain, obtained from the exergy analysis (*Dewulf, j., Van Langenhove, H., 2004*); (2) Minimize the actual energy consumed according to the first law of thermodynamics throughout the production chain; (3) Minimize the amount of greenhouse gases into the entire production chain; (4) Maximize profit or value added; (5) Maximize the possibility of recycling and utilization of waste generated after the end use to generate electricity or produce heat; (6) To maximize the economic value added for any of the alternatives of substitution, recycling or electricity generation or heat.

Scales of measurement will also have to be defined for each criterion.

4) Case study data collection

According to the results of steps 2 and 3, data will have to be gathered in order to perform the analysis.

5) Preference modeling

Using the PROMETHEE methods requires model the preferences of the stakeholders:

- Preference functions have to be associated to the different criteria to
- Weights are allocated to the criteria to represent the priorities of the stakeholders.

6) Model calibration and validation

A complete robustness and sensitivity analysis will be performed to ensure that the multicriteria model is consistent with the preferences of the stakeholders and provides sustainable solutions.

7) General framework definition

The conclusions drawn from the case study will be used to elaborate a general framework for extending the developed methodology to other analyses (other materials, other countries ...).

8) Presentation of the results

The implementation of the results of this research in the energy policies of Belgium and Mexico would help to improve the adoption of measures in the energy and environmental policy in close link with research centers, civil society and companies, offering products and services to ensure sustainable development.

Expected results of the project

Development of a multicriteria methodology for the comparison of alternative solutions for the production of daily-used materials, in the perspective of sustainable development in a long term

The obtained methodology should make it possible to improve energy use efficiency and to reduce environmental impacts such as pollution and waste.

The methodology will be applied in several case studies, mainly in the field of science and materials engineering for the manufacture of end use of different materials. The analysis will be performed from the

simplest (e.g. polystyrene versus cups of ceramic vessels), increasing its degree of complexity (for example, the manufacture of poly (ethylene Terephthalate), PET bottles, versus recycling, or using substitutes such as glass and/or aluminum.

Projects and/or case studies to define must be useful to the Belgian and Mexican industry. Based on the results of the methodology, it will be possible to assess and rank technologies and its evolution.

We have considered the following criteria set for the project:

1. - Technical Criteria

1-1- Material balance of life cycles of every technological process involved in the production chain of the stuff considered.

1-2- Energy balance of life cycle of every technological process involved.

1-3- Energy efficiency indirectly measured through efficient use of energy considering exergy analysis. It will be considered the "Irreversibility" as a measure of energy efficiency.

2. - Environmental Criteria:

2-1- Measure of CO₂ emissions (Greenhouse gases).It will be Included NO_x and SO_x

3. - Economic criteria:

3.1. - Added Value in the whole chain of production.

3.2. - Product value evaluated as the production cost plus Return on Investment (ROI) representative of capital cost.

4. - Social criteria:

4.1. - Effects on employment.

Some results. From the analysis detailed before in this paper, it is considered that a subset of technologies will also inevitably reflect the modes of using energy and its possible changes.

The possible implementation of the results of this research in the energy policies of a specific country would help to improve the adoption of measures in the energy and environmental policy in close link with research centers, civil society and companies, offering products and services to ensure sustainable development.

Case Studies

As a result of the methodological survey was explained before, we have compared:

- Polyethylene bags with other materials, being the best evaluated by the multicriteria Prométhée method, as it is shown in Figure...
- PET bottles:
- Polystyrene cups versus

The goal of these case studies was to compare and analyze the exergetic losses embedded with the production of the materials used in the application of film blown bags (i.e., shopping bags) and PET bottles used mainly to bottled water. For the purpose of this paper, plastic bags are defined as supermarket and retail shopping bags and bottles are considered to be of one liter.

Polyethylene bags and PET bottles functional unit.

Bags functional unit is a repeated use of 300 times for reusable bags, which is the average lifetime, while the other kinds of bags are used only once. Because of the carrying capacity of the plastic bag, the functional unit is taken to be the use of 900 polyethylene bags and 675 paper bags (the number of single use bags to carry goods from a store to home equivalent to the use of one reusable bag were recalculated).

The functional unit of PET study is 1 Kg (26 bottles of 1 L or 1 ton PET, 26,000 bottles of 1 liter. This base of calculation was used for the Exergetic Life Cycle Analysis and the atmospheric emissions.

Material to manufacture bags.

Five types of grocery bags were analyzed, three of them are disposable bags: the commonly used plastic bag made from Low Density Polyethylene; a LDPE bag containing a Pro degrading, unbleached Kraft paper bags and two reusable: a Polypropylene fiber bag and a cotton bag. For the Exergy analysis, calculations were based upon the information in table 2, which shows the assumptions and main characteristics related to every type of bag.

Polyethylene is not biodegradable mainly because it has large molecular weight and its large

molecules cannot enter into the cell of microorganism easily. After many years of research, it has now been established that the mechanism of polyethylene biodegradation, known as 'oxo-biodegradation', involves two stages. They are: (1) abiotic (photo or thermo) oxidation, and (2) microbial biodegradation. In the first stage, polyethylene is oxidized leading to the reduction of its molecular weight significantly.

Also, hydroxyl (OH), carbonyl (C=O) and carboxyl (COOH) groups are introduced into polyethylene chain leading to further oxidation of polyethylene.

Pro-oxidants (Pro degrading) are transition metal ion complexes and they are added to Polyethylene in the form of stearate or other organic ligand complexes. Fe^{3+} , Mn^{2+} or Co^{2+} stearates are the most commonly used as pro-oxidants. Polyethylene that has been oxidized by pro-oxidants will be more susceptible to microbial attack than the initial polyethylene film due to increased hydrophilicity and presence of low molecular weight fragments. (Telmo et al, 2009).

Material to manufacture bottles

The methodology described was applied to the case of PET bottles, having as possible substitute materials for aluminum cans and glass bottles. Use the term "primary materials" to refer to those materials obtained from the raw materials, while the term "secondary materials" is referred to the materials produced in a recycling process.

Characteristic of bags analyzed.

Characteristic of bags analyzed are presented in Table 2.

Table 2. Main characteristics of the bags analyzed.

Composition	DISPOSABLE			REUSABLE	
	LDPE (film grade)	LDPE+ Pro degrading	Unbleached Kraft Paper	PP fiber	Cotton (Unbleached)
Size (cm)	25+15x50	25+15X50	35+10x40	37+10x39	31+21X33.5
Carrying capacity (kg)	3	3	4	9	10
Weight (g) Functional unit (f.u.) Weight f.u. (kg)	5.6 900bags 5.04	6 900bags 5.4	42.6 675bags 28.755	60 1bag 0.06 300times used	90 1bag 0.09 300times used
Expected life (f.u.=functional unit).	single use	single use	single use		

Characteristic of bottles analyzed.

The PET analyzed has an intrinsic viscosity between 0.72-0.84, optimal for a bottle grade resin. Also, the color of PET and glass bottles is clear.

In any case it was considered the labels and lid of containers.

The reference flow of these materials for packaging is shown below:

Table 3. Reference flow of packaging materials.	
Material	Reference flow (tone)
PET	1
Aluminum	2.319

Glass	14.84
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Considerations about bags case study.

The cotton composition was found to be of 94% cellulose, 1.3% protein (%N x 6.25), and 1.2% peptic substances, therefore for the Exergy content of cotton, the relation of NCV to chemical Exergy of cellulose was considered.

The Prodegrading additive was modeled as stearic acid and a small amount of Manganese (Mn) metal to represent the presence of manganese stearate. The bag contains 97% PE, 3% additive. There is no extensive data available on production of stearic acid and on Manganese stearate. Fertilizers considered are urea, K_2O_5 and P_4O_{10} .

Considerations about bottles case study.

The raw materials in the PET production are Terephthalic Acid and Ethylene glycol, the first compound is obtained from the crude oil refining, and the second compound, from natural gas processing in a cryogenic plant.

The aluminum is mainly composed of bauxite mineral which in turn contains other minerals such as gibbsite ($Al_2O_3 \cdot 3H_2O$), boehmite ($\gamma-Al_2O_3 \cdot H_2O$), and impurities among which are kaolinite ($Al_2Si_2O_5(OH)_4$), hematite (Fe_2O_3), and goethite ($\alpha-FeO(OH)$), although these impurities are negligible.

The raw materials in the glass production are SiO_2 , Na_2CO_3 , $CaCO_3$, and feldspar.

Taking Mexico's consumption of plastic bags and bottles, we have dimensioned the pollution problem, the energy degradation and the hydrocarbon waste.

In Mexico it was consumed a mean of Polyethylene high and low density, it is approximately of 600,000 ton/year. Considering that 900 bags are equivalent to 5.04 Kg, this is equivalent to 107,100 million bags/year. The gross benefit for producers are about 2 US\$/kg. It means a good business. From the point of view of non-renewable resources waste, in Mexico are scrapped an equivalent of 8.25 million US\$/day (considering a crude oil international price of 84 US\$/barrel).

Taking as base bottles of 1 liter, Mexico has produced 9,760 million of bottles/year. In this case the gross margin benefit is more or less 0.050 US\$/bottle. Only 10% of these bottles are really recycled effectively. As a consequence there is an important world surplus of raw material, i.e. Poly (ethylene Terephthalate). This implies that recycling business needs a special strategy for long term substitution. Bottles scrapped are 9,760 million equivalent to 3,579 million US\$/year.

If technology strives for sustainability, high exergetic efficiency compromises boundary uses of technology. This efficiency is better understood by reducing resource consumption. On the other hand, efficiency is improved through maximizing the exergetic product output with minimization of waste and irreversibility production.

Based on the advantages of Exergy analysis, especially for resource use, we investigate Exergy as a tool in assessing the industrial reutilization or recycling of waste plastics as those related in this paper. It is more or less obvious that recycling or co-generation of electric and heat through incineration may contribute to sustainability comparing it with disposing them into the environment.

Starting with non-renewable resources the overall plastics production coming from oil or natural gas including all the chain production, can be calculated the Cumulative Exergy Consumption (CE_{ExC}).

PE bags vs. alternative materials bags.

Table 3 summarizes the input and output flow of Exergy during these selected production processes for the PE and possible substitute bags. In such way, it has been possible to identify the life cycle steps with the

main Exergy losses due to the process irreversibility and to the environmental pollutant releases.

Low Density Polyethylene was produced by a high pressure process autoclave reactor. This gives a total of Exergy losses of 244.005 MJ/f.u. for the total Polyethylene production. Considering the characteristics of composition of oxo-degradable bags (97% LDPE and 3% additive), the total Exergy losses for polyethylene degradable bags are 259.6 MJ/f.u. As for bags made of unbleached Kraft paper, the total Exergy losses for this process are 3492.576 MJ/f.u. In the case of reusable bags, the life cycle of Polypropylene, manufactured by a bulk slurry phase loop reactor process, presents a total of 2.018 MJ/f.u. exergy losses. On the other hand, we found a total of 292.73 MJ/f.u. of exergy losses for the cotton bags.

Total Exergy outputs do not take into account Exergy of emissions since they are considered as losses, therefore emissions are not considered for the calculation of irreversibility related to the processes. Although other emissions to air, water and soil are not included. CO₂, methane, SO₂ and mostly CO₂ emissions are the main substances related to pollution.

Table 3 illustrates the results of the Exergy analysis, which represents the Exergy destruction by process irreversibility associated with each production stage on the life cycle of the examined materials. As can be seen from the columns, the production of unbleached Kraft paper destroys the highest quantity of Exergy, which represents a much more relevant input than PE bags from the viewpoint of Exergy consumption. Table 4 shows the emissions embedded within the life cycle of the alternatives analyzed.

Table 4. Exergy flow of the different alternatives for shopping bags all in MJ/f.u.

	DISPOSABLE			REUSABLE	
	LDPE (film grade)	LDPE+ Pro degrading	Unbleached Kraft Paper	PP fiber	Cotton (Unbleached)
Exergy Inputs	933.733	952.33	4054.086	19.0984	294.491
Exergy Outputs	689.728	692.7089	561.51	17.08	1.757
Irreversibility Emissions	236.527	251.5312	3484.78	1.887	292.623
	7.478	8.0899	7.796	0.1314	0.111
Total Exergy losses	244.005	259.6211	3492.576	2.0184	292.734

Table 5. CO₂ emissions for the alternatives for bag manufacturing.

Material	kg CO ₂ /f.u.	MJ/f.u.
LDPE (film grade)	16.559235	7.478
LDPE+ Pro degrading	17.9142224	8.0899
Unbleached Kraft Paper	17.2634122	7.796
PP fiber	0.29097131	0.1314
Cotton (Unbleached)	0.24579768	0.111

The production of low density polyethylene bags with an oxo-degrading additive has the highest Exergy embedded in emissions. From table 4, it is clear that the production of 1 polypropylene

bag that is equivalent to the use of 900 PE bags, involves the lowest losses of Exergy. These data suggest that the employment of alternative materials instead of Polyethylene for the production of retail shopping bags is not always the best choice, even if the material inputs are lower between the functional units like is the case of cotton reusable bags. At the end of its first use, PE and PET can be simply disposed in the environment without any conversion. Alternatively, they can be converted through incineration or through landfilling with methane capture for heat and/or electricity production. They also can be recycled resulting in the same plastics if it is possible. Of course recycling systematically generates the highest output. In the case of Polyethylene it is only possible to recycle 60% in the best case.

PET bottles vs. alternative bottle materials.

We have performed the calculations for PET manufacturing process from Terephthalic acid and ethylenglycol considering the input-product coefficient of PEP (Process Economic Program). Table 6 shows the chemical exergies with their irreversibility along with the atmospheric emission of PET manufacturing and their respective chemical exergies. Table 6 shows the exergy flows of PET bottles production.

Table 6. Exergy Flow of PET Manufacturing Process from Terephthalic Acid and Ethylenglycol

Production of Terephthalic Acid			
	Input (MJ/uf)	Output (MJ/uf)	Irreversibility (MJ/uf)
*Xylenes	674,864	614,266.91	60,597.09
p-xylene	40,241	26,545	13,696
Terephthalic Acid	45,585	18,122	27,463
Irreversibility of Terephthalic Acid: 101,756.09 MJ/uf			
Production of Ethylenglycol			
	Input (MJ/uf)	Output (MJ/uf)	Irreversibility (MJ/uf)
**Ethane	45,130	44,895	235
Ethylene	18,716	10,843	7,873
Ethylene Oxide	24,402	6,693	17,709
Ethylenglycol	8,936	7,510	1,426
Irreversibility of Ethylenglycol: 27,243 MJ/uf			
PET	29,873	23,705	6,168
Bottles	34,885	23,705	11,180
Irreversibility of bottles production: 17,348			
Total irreversibility of PET bottles: 146,347 MJ/f.u. (24.5 bpce/uf)			

Glass Bottles

The results of glass bottles are presented in the Table 7, considering the same variables, i.e. exergy and energy balances including of course total irreversibility and GHE. The functional unit is also an equivalent of 26,000 one liter bottles.

Table 7. Exergy Flows glass bottles production.

Process	Exergies		Irreversibility (MJ/uf)
	Input (MJ/uf)	Output (MJ/uf)	
SiO ₂	8,207	445	7,762
Na ₂ CO ₃	17,237	1,450	15,787

CaCO ₃	1,704	674	1,030
Feldspar	2,057	304	1,753
Glasscasting	52,023	2,582	49,441
Bottlesblowing	20,390	2,582	17,808
TotalIrreversibility ofglassbottlesproduction:93,581MJ/fu			

Aluminumcans.

Itisalsoconsideredthesamevariables: exergycalculationstoobtaintheirirreversibility ineach productionstep. Thefunctional unitisalso26,000bottlesofone liter.

Theresultsof glassbottlesarepresented inTable8.

Table8.ExergyFlowsglassbottlesproduction.

Process	Exergies		Irreversibility (MJ/fu)
	Input (MJ/uf)	Output (MJ/fu)	
Bauxite	5390	2746	2,644
Alumina	17300	675	16,625
Coke	55,017	36,754	18,263
Na ₂ CO ₃	7,756	476	7,280
CaO	2,747	630	2,117
NaOH	20,273	11,719	8,554
Electrolysis	170,563	76,295	94,268
Cansproduction	78,375	76,295	2,080
TotalIrreversibility ofcansaluminum production:151,831MJ/fu			

Itisimportant toremember that anotherimportant alternative tosubstitute PETbottlesproduced fromoil andgasasrawmaterialsistouse recyclePETbottles.Thesame treatment isapplied forglassandaluminumbottles, i.e. recyclingprocessesfor eachoneof them.

Oncecalculatedthetotalirreversibilityofthematerialsinprimaryandsecondaryproduction,we present thefollowinginasummarytable9:

Table9.Irreversibilityinbottlematerials

Irreversibility(MJ/fu)		
Material	Primaryproduction	Recycling
PET	146,347	13,037
Glass	93,581	53,688
Aluminum	151,831	8,416

Thefigure6showstheirirreversibilityfor the PET, glassandaluminumbottlesconsideringits primaryandsecondaryproduction,it ispossible toconsider that therecyclingaluminumcans minimize theirirreversibilitybetter than PETandglassbottles. However,theirirreversibility in the recyclingPETbottlesis important witha reductionof136,334MJ/fu.

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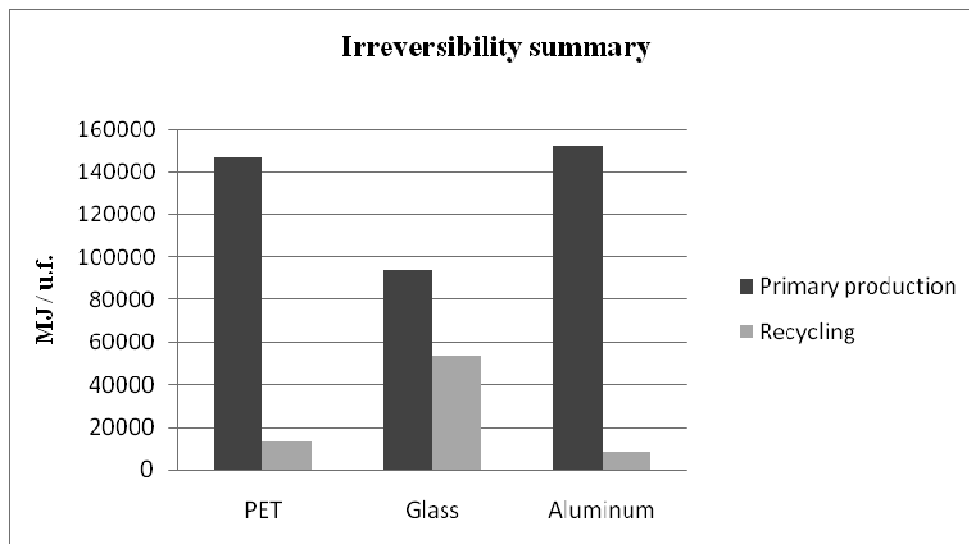


Figure6 Irreversibilitysummary.

Multicriteria decision making.

In the end of the methodology that has been presented above, we will use PROMÉTHÉE-GAIA Multicriteria decision aid method.

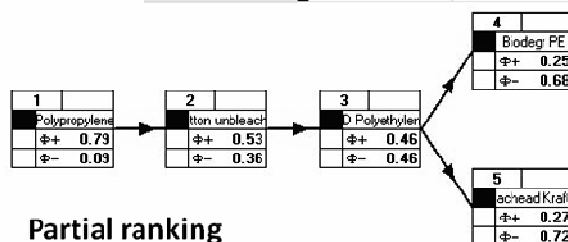
Then for taking a decision about the substitute materials or the recycling process, they should be measured with various criteria, using as a case study the Mexico's poor development in sustainable issues.

Multicriteria results for bags case study.

Then for taking a decision about the substitute materials or the recycling process, they should be measured with various criteria, using as a case study the Mexico's poor development in sustainable issues:

- Minimize process irreversibility in the whole Life Cycle.
 - Minimize non renewable resources used in its Life Cycle.
 - Minimize real quantity of energy in each one of the processes involved in the Life Cycle of all alternatives.
 - Maximize end product value [total cost of production plus 25% on Return on Investment.
 - Minimize GHG in the whole life cycle of each alternative.
 - Using the results of each variable calculated according to our methodology, we present the results of Multicriteria solver *DecisionLab*, as follows (Figure 7).
- According to the ranking obtained by PROMETHEE, the bags made from Propylene and Cotton are:

Decision Lab - [Bags1]				
File Edit View Insert Tools Window Help				
Scenario1				
	Irreversibilit	Real energy con	Mass balance LCA	Product value
Min/Max	Minimize	Minimize	Minimize	Maximize
Weight	1.2801	1.0000	1.1975	0.5223
Preference Functi	V-Shape	V-Shape	V-Shape	Gaussian
Indifference Thres	-	-	-	-
Preference Thres	2.0000	2.0000	0.0050	-
Gaussian Thresho	-	-	-	133.2400
Threshold Unit	Absolute	Absolute	Absolute	Absolute
Average Perform	853.4694	170.5980	0.1144	133.2460
Standard Dev.	1475.3377	253.6512	0.1210	170.7293
Unit	Mega Joules	Mega Joules	barrels of pce	Mex \$/ton
LD Polyethylene	236.5270	110.6000	0.2070	118.0000
Biodegr PE	251.5300	120.9400	0.2700	126.0000
Unbleached Kraft	3484.7800	613.1700	0.0905	419.0000
Polypropylene	1.0670	2.0000	0.0035	1.3000
Cotton unbleached	292.6230	5.4720	0.0009	1.9300



Partial ranking

the best material based on the criteria considered (Irreversibility, real energy, mass balance, and unit product value). Taking into account as another criterion GHG, (Green House Gases), mainly CO₂ during the whole LCA, the results have changed taking into account the preference order; nevertheless the bags made from polypropylene are always the better alternative.

Multicriteria results for bottles case study.

The criteria used in decision making through Decision Lab software were:

- Total Irreversibility (MJ/fu)
- Energy consumption (MJ/fu) to be interpreted also as measure of natural resources.
- GEI emissions (Ton.CO₂eq)
- Economic gains (\$/fu)

The alternatives studied are divided into two groups, bottles coming from primary materials (virgin) and secondary materials (recycled) for each one of the three types of packaging materials considered.

The overall comparison between the two groups of materials is shown in the next figure 8 with the next ranking:

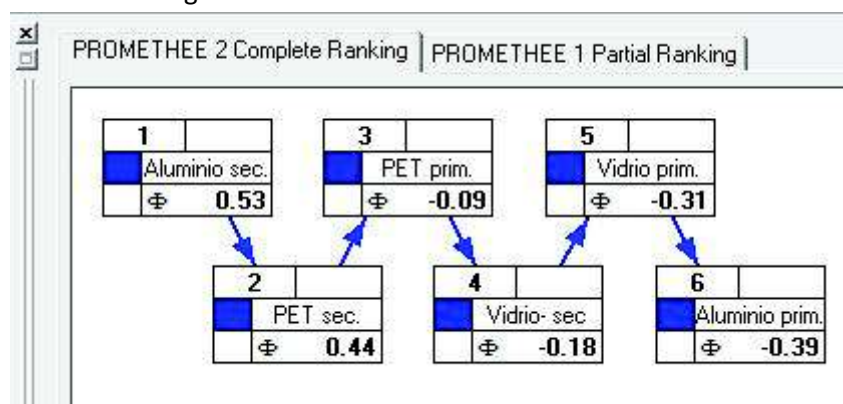


Figure 8. Ranking obtained from PROMETHEE II for primary and secondary materials.

It is possible to see that recycling has a higher order to meet the goal of sustainability. Indeed, the two best materials for recycling are aluminum cans and PET bottles, in this order of priority. Glass recycling is not competing with the other materials because it presents a negative net flow of preference.

We use the formation of two clusters. One is named "primary cluster" signifying that all materials are manufactured from their primary resources. The second one is called "secondary cluster" because all materials within it are manufactured by recycling bottles obtained from the primary cluster.

Using PROMETHEE-GAIADecision-Lab software we have obtained the following results.

The ranking for primary materials: PET ($\Phi=0.19$) > Glass ($\Phi=0.05$) > Aluminum ($\Phi=-0.24$).

The ranking for secondary materials: Aluminum ($\Phi=0.58$) > PET ($\Phi=0.42$) > glass ($\Phi=-1.00$).

In the primary materials, the aluminum cans compete to a lesser extent due to an energy-intensive process in the electrolysis process. However, in the recycling process, the aluminum is the best material according to the criteria used.

The secondary PET is also a good alternative to a second position located not far from secondary aluminum. In the recycling process, glass bottles are in last place with a negative preference flow, so there is less competition.

From the above solutions with the PROMETHEE methodology, it is possible to set a combination of different substitution strategies that should be analyzed from the point of view of supply of raw

materials. Accordingly, the strategy formulated in this study was to replace the growth rate of PET (10%/year) gradually from 2016 to 2035. Thus, in the 2035, the amount will be

replaced is 406,692 Ton/year, of which half will correspond to secondary aluminum and the rest to secondary PET. In other words, 5% of growth rate of primary PET will be replaced by secondary aluminum and the other 5% by secondary PET. In the next table 10 the strategy is shown:

Table 10. Substitution strategy.

Irreversibility, Energy and TonCO ₂ eq.						
	Irreversibility (million boce)		Energy (million de boce)		Million de tonCO ₂ eq	
	Without Replacement	With Replacement	Without Replacement	With Replacement	Without Replacement	With Replacement
21	28.9	26.20	14.6	13.31	6.5	5.94
26	46.5	42.15	23.5	21.39	10.5	9.59
30	68.2	61.82	34.4	31.31	15.4	14.07
35	109.8	99.52	55.4	50.43	24.8	22.66

Polystyrene cups versus porcelain mugs.

This case study compares porcelain mugs as a condition to use efficiently the energy, considering the use 3000 times a mug produced with the silica in a four feed with natural gas and the necessary electricity for washing the mugs in a machine and the use of 3000 polystyrene cups produced from crude oil.

The flows in the exergy analysis are:

Components	PS cup	porcelain mug
coal	0.378	4.700
crude oil	23.600	
natural gas	0.685	7.478
oxygen	63.961	34.615
phosphate		0.045
total	88.624	46.793

565

And the flows out were:

Components	PS cup	porcelain mug
CO ₂	55.100	29.600
H ₂ O	26.520	14.773
SO ₂	0.428	0.066
PS waste	6.115	
NO	0.304	0.172
N ₂	0.020	1.701
ash	0.032	0.395
CO	0.023	0.021
C _x H _y	0.081	0.023
CH ₄		0.043
phosphate		0.045
total	88.624	46.793

566

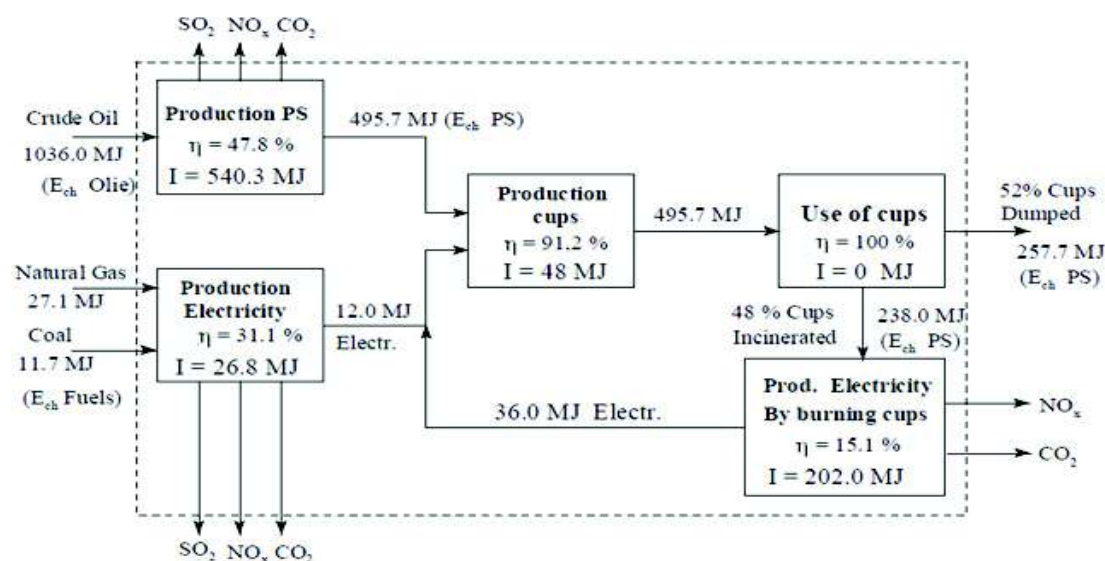
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The following diagrams show the exergy analysis of the entire life cycle of each material.

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Figure Exergy diagram of the life cycle of 3000 disposable PS cups.

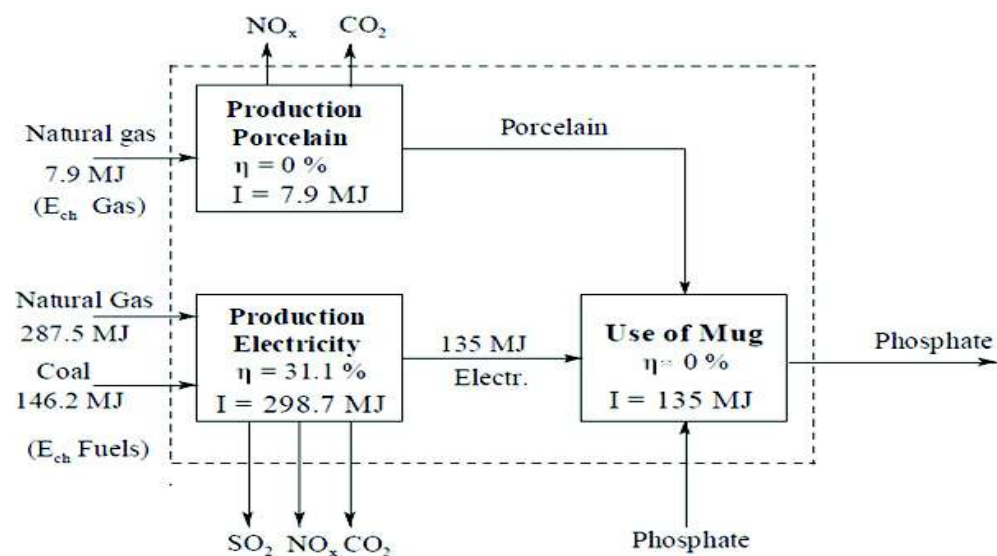


Figure Exergy diagram of the life cycle of the porcelain mug.

Bio based chemicals.

On the other hand, one of the new alternatives coming from Prospective methodology were to evaluate is Biopolymers divided in a lot of potential products and technologies.

Sustainability also means take into account significant steps to move from today's fossil based economy to more sustainable one, based on biomass. There we will find estimating technical substitution potential products to compare in a multicriteria fashion with actual materials considered to satisfy human needs.

As an example of chain valued of biopolymers, Figure shows the great quantity of possibilities.

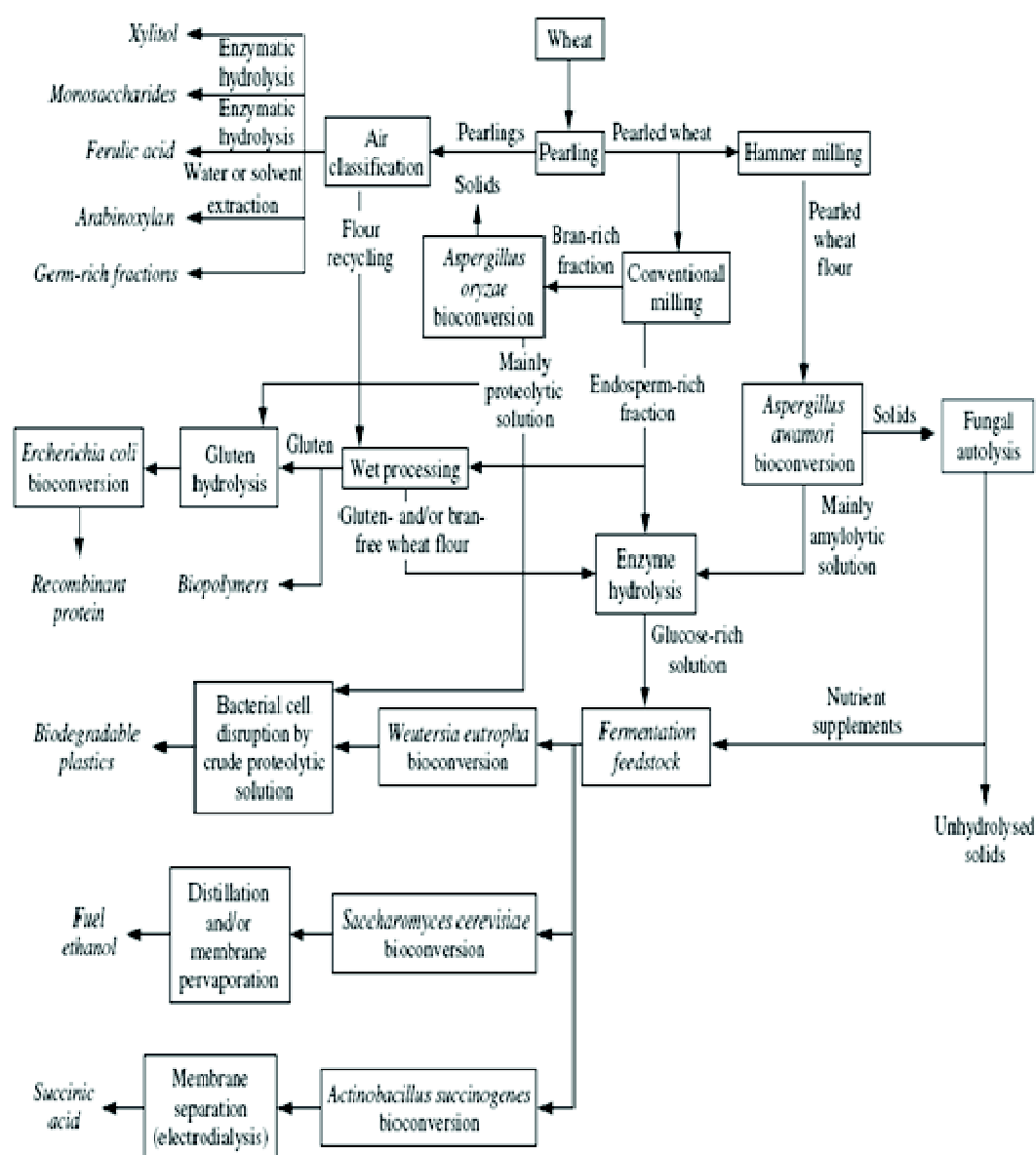


Figure Proposed Wheat-based bio refining strategy for replacing the conventional wheat dry process to obtain biopolymers.

The transition to a bio based economy has multiple drivers:

- The need to develop an environmentally, economically and socially sustainable economy.
- The anticipatory reaction about oil, gas and coal will reach peak production in a more or less short future, considering these resources as the raw material to produce petrochemicals and then final products as those we want to substitute considering the multicriteria assessment methodology.

- The need to reduce atmospheric greenhouse gases (GHG) emissions.

- The necessity to stimulate regional and agricultural development.

A key factor in the realization of a successful bio based production will be the development of biorefinery allowing highly efficient and cost effective processing of biological feedstocks to a range of bio based products. [IEA Bioenergy Implementation Agreement, task 42, 2008].

Industry is increasingly viewing chemical and polymer production from renewable resources as an attractive area of investment. Within the project of a Biorefinery there are significant opportunities for development bio based building chemical blocks (chemicals and polymers) [IEA Bioenergy Task 42 Biorefinery].

There exists a classification approach about four main features which are able to classify and describe a biorefinery system:

1. Platforms as core intermediates (C₅-C₆ hydrocarbons, syngas, lignin, pyrolytic liquid).
2. Products: Energy carriers, chemicals and other products.
3. Feedstock as biomass, from production or residues from forestry, agriculture, aquaculture.
4. Processes as thermochemical, chemical, biochemical and mechanical.

The platforms are the most important feature in this approach; they are key intermediates between raw materials and final products, and can be linked to understand different concepts and targets markets.

The platforms range from single carbon molecule such as biogas or syngas to a mixed C₅ and C₆ hydrocarbons derived from starch, sucrose or cellulose, liquid oils (plant or algal), organic solutions from grasses and pyrolytic liquids. The primary platforms can be converted into a wide range of final products as in the actual petrochemical industry (Escobar,) is made. In the biorefinery case, it is needed a mixed of thermal, biological and chemical processes.

The economic production of biofuels and therefore (petro) chemicals, mainly polymers is still a challenge. The coproduction of chemicals, materials feed should generate the necessary added value.

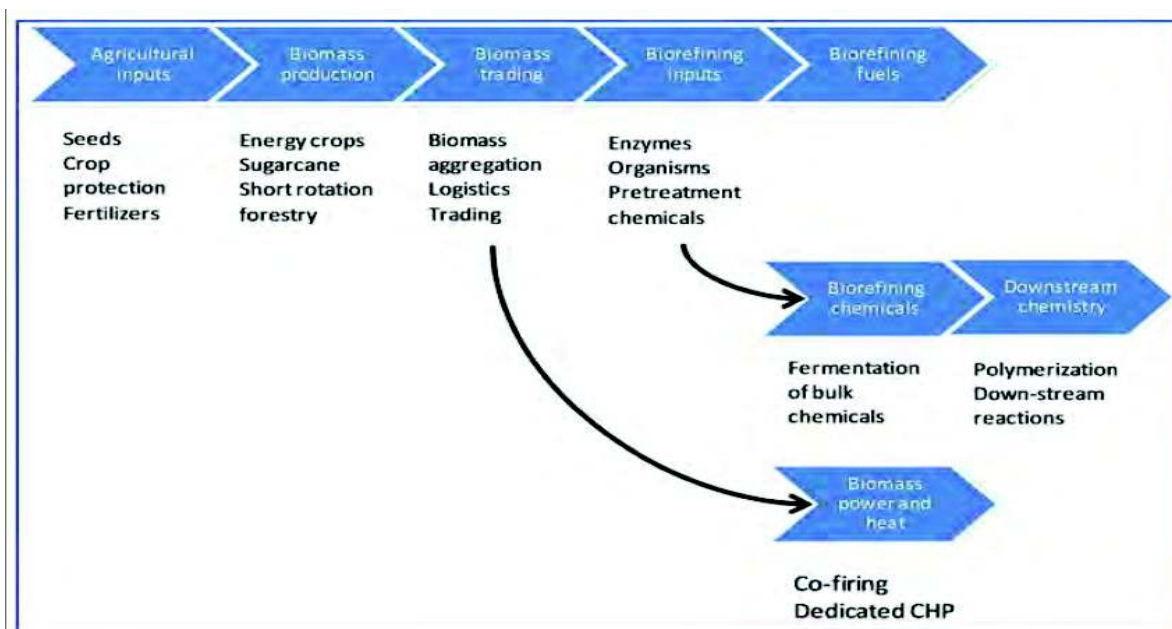


Figure .An example of bio-based products value chain.

In order to really innovate, the following step was performed: Bio-based chemicals and bioenergy production, being the motivation,

•**Bioenergy** and **bio-based chemistry** are fostered in European Union.

- A 20 % renewable share of EU final energy consumption by 2020 and a 10 % share in transport sector specifically.
- European Chemical Industry Association set a 15 % incorporation target of renewable feedstock by 2017
- These sectors are facing many uncertainties: Competition within conventional biomass uses. Many production pathways proven at pilot scale; change in regulatory framework.

The Bio-based chemistry impact on bioenergy sector Methodology has some assumptions to notice:

Fossil fuel prices are consistent with IEA's WEO 2010 « New Policies » scenario

Feedstock availability and cost consistent with 2000-2010 baseline

No importation of commodities

Advanced technologies costs divided by 2 in 30 years

The solution strategy could be:

1)Bio-based chemicals are produced in priority

2) Then, bioenergy production is incrementally increased until feedstock shortage

If we assess the bio-based chemistry demand motivations some conclusions could be as follows:

- Top-down approach for the 7 main « building blocks »

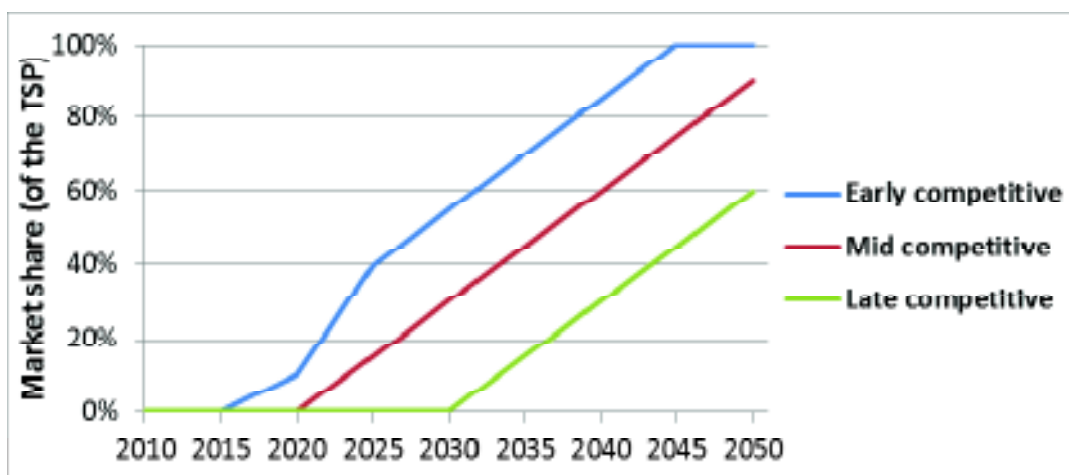
1. Projecting future demand: **Two scenarios : consumption annual growth rate of 0.5 % and 2 %**

2. **Estimating technical substitution potential (%) as follows:**

Ethylene	100
Methanol	100
Propylene	100
Butadiene	75
Benzene	75
Toluene	75
Xylenes	100

3- Estimating bio based market development

The estimation of based market development can be seen in the following graph:



Some conclusions about bio-based chemistry and bioenergy are:

- Bio-based chemistry could have an impact on bioenergy sector: Reduction of 3 Mtoe in the **low** bio based development scenario; Reduction of more than 5 Mtoe in the **high** development

scenario. The new regulatory framework could lead to a slight increase in total bioenergy production. But, it could lead to a biofuel production decrease, especially combined with a high bio-based chemistry demand. The competition between uses shall need an adequate regulatory framework to respect the use ranking and to not threaten conventional uses.

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