THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING

ENVIRONMENTAL ASSESSMENT OF EMERGING TECHNOLOGIES

THE CASE OF BIOPOLYMERS

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Göteborg, Sweden, 2006

[...] les opinions des hommes sont receues à la suitte des creances anciennes, par authorité et à credit, comme si c'estoit religion et loy. On reçoit comme un jargon ce qui en est communement tenu ; on reçoit cette verité avec tout son bastiment et attelage d'argumens et de preuves, comme un corps ferme et solide qu'on n'esbranle plus, qu'on ne juge plus. Au contraire, chacun, à qui mieux mieux, va plastrant et confortant cette creance receue, de tout ce que peut sa raison, qui est un util soupple, contournable et accommodable à toute figure. Ainsi se remplit le monde et se confit en fadesse et en mensonge.

[...] for mens opinions are received after ancient beliefs by authority and upon credit; as if it were a religion and a law. What is commonly held of it, is received as a gibrish or fustian tongue. This trueth, with all her framing of arguments and proporcioning of proofes, is received as a firme and solid body which is no more shaken, which is no more judged. On the other side, every one the best he can patcheth up and comforteth this received beliefe with all the meanes his reason can afford him, which is an instrument very supple, pliable, and yeelding to all shapes. 'Thus is the world filled with toyes, and overwhelmed in lies and leasings.'

(Montaigne, *Essais, 1595*)

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Abstract

Current efforts to mitigate climate change, using renewable resources and reducing waste, drives the development of new industrial processes. In this study we examine the technologies for conversion of biomass to plastics. There are basically two types of processes: the biotechnology based ones, some of which are commercially available and the thermochemical process ones we looked into in more detail. Indeed, the latest process routes, based on gasification and synthesis gas technologies, are potentially technically feasible, since all process units are currently either commercially available or in the pilot plant phase. In the study their economic and environmental feasibility are evaluated.

We evaluate the environmental attractiveness of this emerging technology using life cycle assessment (LCA) methodology. Both final environmental and economic evaluation are based on process modeling of the biomass to plastics route. The outcomes of the study are the environmental and economic assessments as such, but also a contribution to the on-going efforts to integrate LCA with process modeling and economic tools. We also expect to contribute to methodology development through the collection and documentation of feedbacks from environmental assessments of new, emerging technologies.

Keywords: biopolymers; life cycle assessment; biopolymer, environmental assessment; cost assessment; process modeling

List of publications

Appended papers

Paper I:
Waste to plastics: process alternatives:
Selim Nouri, Kristin Kaggerud and Anne-Marie Tillman

(Submitted for publication: Biomass and Bioenergy)

Paper II:
Making Technology screening useful for Life Cycle Assessment:
The Case of Bioplastics
Selim Nouri

(Submitted for publication: Journal of Industrial Ecology)

Other publications by the author

Nouri, Selim and Anne-Marie Tillman (2005) "Evaluating synthesis gas based biomass to plastics (BTP) technologies". CPM - Centre for Environmental Assessment of Product and Material Systems, Chalmers University of Technology, Göteborg, CPM report 2005:6

Nouri, Selim and Kristin Kaggerud (2006). “Waste-to-plastics: process alternatives”. CPM - Centre for Environmental Assessment of Product and Material Systems, Chalmers University of Technology, Göteborg, CPM report 2006:10

Nouri, Selim (2005). “Biomass to polymers (BTP)”, Poster. AGS Research Partnership: New Materials for Sustainable Development. AGS, MIT, Cambridge, March 2005

Nouri, Selim (2005). “EVALUATING SYNTHESIS GAS BASED BIOMASS TO POLYMER (BTP) TECHNOLOGIES”. Life Cycle Management conference, Barcelona, Spain September 2005.

Nouri, Selim, Kaggerud, Kristin, Tillman, Anne-Marie (2006). Combining Life Cycle Assessment (LCA) and process modeling. FZK Material Design and System Analysis International workshop, Forschungszentrum Karlsruhe (FZK), 16th may 2006, Karlsruhe, Germany.

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Contents

1 Introduction

1.1 Project start: new materials for sustainable development.

Our world is facing many challenges like increasing waste flows, resources depletion and climate change. For each sector, alternative strategies and technologies have been studied and for the material sector, biopolymers are one of them.

However, evaluating the impacts on sustainability (impact on energy use, emissions, and resources) over the entire materials cycle for emerging biopolymer is decisive for early design phase and product development. Questions regarding the capacity of bioplastics to solve the inherent problems of their fossil based counterparts and the technical feasibility as well as the financial coherence of biopolymers projects have to be answered before any decision is made.

Much work has already been done about biopolymer materials; however, we will try to integrate together technical feasibility (through chemical process modelling), environmental and economical aspects together. This is the background of our project[1] and the starting point of our research on bioplastic production processes and their environmental impact as well as their financial feasibility.

1.2 Purpose

The purpose of this project is to contribute to the improvement of sustainability[2] assessments of emerging technologies – in our case bioplastic production – and by applying environmental systems analysis tools like LCA and cost assessment methodologies to a specific case study like bioplastics, to get some feedbacks regarding the best way to do so and to contribute to a more general methodology in the field of sustainability assessment of emerging technologies.

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[1] The project background is an AGS-CPM project named new materials for sustainable development where a research partnership between MIT, Chalmers, UT and ETHZ have been working on different case-studies to develop an integrated method for assessing new material substitution issues. It was during this project that the case study of sustainable plastics was chosen and that partnership between MIT and Chalmers was strengthened. The first cost analysis and environmental assessment were performed during this partnership period (2004)…

[2] We will focus mainly on environmental and cost assessment in this study.

Concretely, the specific purpose of our work is to assess environmentally and economically, routes towards bioplastics that are potentially feasible but that have not been industrially implemented and get some feedbacks regarding methodology.

Ultimately our project target is to provide optimizing decision-making tools.[3] We will try to design and provide increasingly more pro-active/re-active[4] and precise tools for measuring progress towards sustainability in the emerging technologies field (e,g. bioplastics), for assessing the environmental and financial impact of specific actions - like early technology investments - or products, supporting long-sighted decisions, aligned with other business objectives, turning environmental issues into opportunities. Our case study for experimenting those tools is a bio-based polymer process.

1.3 Research plan

The research we have done regarding bioplastics was roughly following the diagram hereafter:

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[3] An example of such ultimate decision making tool would be a process modeling software that includes cost assessment, environmental impact assessment and regulations in the same package, setting maximum emissions factor as a constraint to the design of the process. Ultimately, environmental data and regulation could be updated on-line as it is the case today with economic data (like spot prices of raw materials and electricity costs).

[4] The tendency today is to develop pro-active tools and strategies (long term perspective, planification) whereas re-active tools are often seen as “bad” because of the passive connotation they embed with them. However it is here a fundamental remark to ask: “are re-active tools and strategies that bad?” Or even: “are not they what we precisely need in those times of high unpredictability (oil price, climate change)?” A good metaphor here is the one of the eagle and the bat: whereas the eagle (pro-active and long-sighted) has an average pray rate of 9 %, the bat (re-active and short-sighted with its biosonar) has a capture success of about 35%. Therefore, re-active tools that allow quick and simple responses to complex environmental problems may be not that bad. Moreover, in a worst case scenario where for instance a very big environmental problem (like climate change) may be irreversible, re-active tools and strategies may be much more useful than obsolete long term and pro-active ones. Adapting ourselves to change, if unable to prevent it, may be a – the only? – good option for survival .

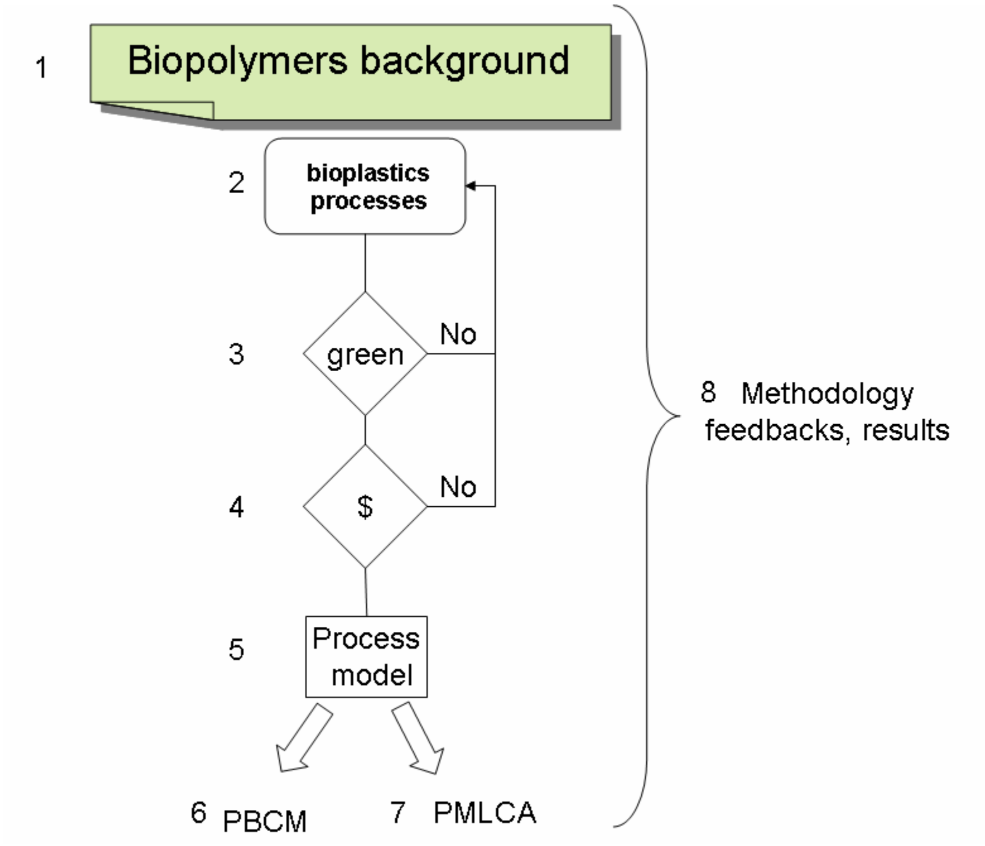

Figure 1: Research plan diagram

First of all we looked at the biopolymer background (1, figure 1) using a list of relevant issues that should be considered when dealing with bioplastics. This list of issues includes a variety of subjects like bioplastic performance compared to actual plastics, market tendencies, etc. This is important to understand before going into further detailed environmental assessment. Then, after having identified the different technologies that can potentially lead to bioplastics (2, figure1), we followed a relatively simple procedure: once having selected a process we assessed its potential environmental impact using a simple environmental assessment tool, stream-lined LCA (3, figure 1). If the process is environmentally friendly – compared to fossil fuel based counterparts – then a simple cost assessment is performed (4, figure1). If the process is not “green” enough, we pick a new one. If the cost assessment is conclusive – compared to existing bioplastics – we go to the next step of process modeling (5 in figure 1). If the cost is too high, we pick up another production route. If both environmental assessment and cost assessment are encouraging, a more detailed process model is made. When a process model of the route is made - this process model can be greatly enhanced by using HYSYS or other process modeling softwares – it is then used to have better performance assessments method regarding both cost and environmental impact. For process model based cost assessment, MIT's Process Based Cost Modeling (PBCM see 6 in figure 1) can be used; and for process model based environmental assessment, Process Modeling Life Cycle Assessment (PMLCA see 7 in figure 1) can also be employed. Finally, we present relevant results from the study and some methodology feedback regarding the environmental assessment of emerging technologies (see 8 figure1). This is what is going to be presented here and the structure of this thesis will follow this research plan.

The thesis structure is the following: in a first part we will present and discuss the biopolymer background and related issues, then we will present a chosen bioplastic production route and its environmental impact via a stream-lined LCA. This will be followed by some assessments of the cost of production and its variation with the production capacity. Then the process modelled based assessments will be presented with first the process based LCA and then some comments on the MIT's Process Based Cost Modeling (PBCM) method and an example of labor factor calculation via process modeling. After that, discussion about the biopolymers in general, sustainability results and methodology feedbacks will be presented. Finally conclusions will be presented.

Let us start now with the biopolymers background.

2 Biopolymer background

Before going to more details regarding sustainability assessment, we will now present a listing of important issues regarding bioplastics to have a clearer perspective from the biopolymer background.

Indeed, to understand correctly environmental assessments of new technologies and especially the case of bioplastics, a wider horizon than just techno-economical or environmental research is needed. Indeed, technological choice, economical trends as well as acceptance issues are crucial to understand biopolymers's environmental assessment and to improve the quality of those assessments for emerging technologies. The intention is to present the main issues that need to be understood. A market perspective is used in the sense that the different applications of biopolymers is discussed. In addition, different ways to measure sustainability, in terms of what aspects are considered important, is presented.

We will start by presenting general issues like the global biomass potential and bioplastics abilities to solve problems and then describe what kind of research could be done regarding sustainable assessment of biopolymer.

2.1 General background

2.1.1 Identification of potentials of the biopolymers to solve environmental and resources problems and possible new issues

It is crucial to go through this pitch step before going further into sustainability assessments since it gives us an overview of the pros and cons of new bioplastic technologies.

Producing biopolymers could:

- solve the plastic littering problem
- save fossil fuel[5]
- decrease green house gases emissions
- decrease transport of environmentally harmful substances like oil
- save energy (regarding bioplastics new issues, one could notice that it is quite strange that decreasing oil transport and thus risk of

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[5] The situation regarding fossil fuels and particularly natural gas is a paradox in itself (see appendix 1)

oil spills is not more widely used as a main argument to promote bioproducts).
- decrease sulphur emission and desulphurisation cost for fuel production (low sulphur content of biomass compared to coal, oil and gas)
- increases dedicated new waste management systems of bioproducts (like composting or gasification)

Possible new issues potentially being introduced are:

- biodiversity threat by using extensive short rotation dedicated crop
- nutrients and ashes recycling in case of wood waste use as feedstock.
- technology evolution/transition. For instance, the introduction of bioplastics with lower energy content compared to classic polyolefins in an incineration based waste management system could hypothetically indirectly increase on a short term perspective the global output of CO2 emissions[6] (see figure 2). This is typically a matter of technology evolution and this phenomenon has already been studied for solar cells (Sandén 2004).

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[6] "Using plastics means protecting the climate! ..//.. By using plastics waste as an alternative to traditional fuels such as coal for power generation, for example, greenhouse gas emissions are reduced by 20-25%. A recent study has estimated the effects on climate change if plastics were to be replaced by alternative materials wherever possible across the whole of Western Europe. The results indicate that there would be an additional energy requirement of around 10%, or about 25 million tonnes of crude oil, corresponding to 105 million tonnes of CO2 greenhouse gas emissions per year. This is equivalent to a third of the Kyoto reduction target for EU-15 countries. It is not unreasonable to suppose that the continuing growth of plastics in both existing and new applications will also enhance the energy efficiency of products and services, and therefore continue to contribute to reducing the climate change effects related to products required by society. Plastics can play an important role alongside other developments and initiatives in ensuring that our future is indeed sustainable". (PlasticsEurope 2006)

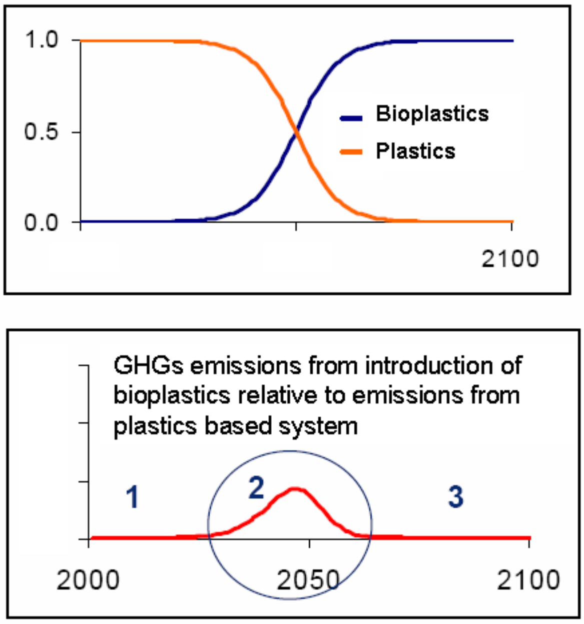


Figure 2: Potential development of greenhouse gas (GHG) emissions during a transition scenario towards bioplastics. In period (1), the proportion of bioplastics produced is so small that the emissions are negligible. In the transition period (2), because of their lower energy content, when introduced in the existing incineration system, the global emissions are increased (see PlasticEuropes comments in footnote 6, p5) and at the end, when all plastics are replaced by bioplastics (3), there are no more emissions due to the carbon neutrality of the system. Different scenarios can be drawn to explain this phenomenon (Sandén “Technology assessment and future studies: change of backgrounds systems” 2004, adapted).

2.1.2 Establishing the sources and availability of raw materials

Biomass resources are significant (see energy balance, figure 3).

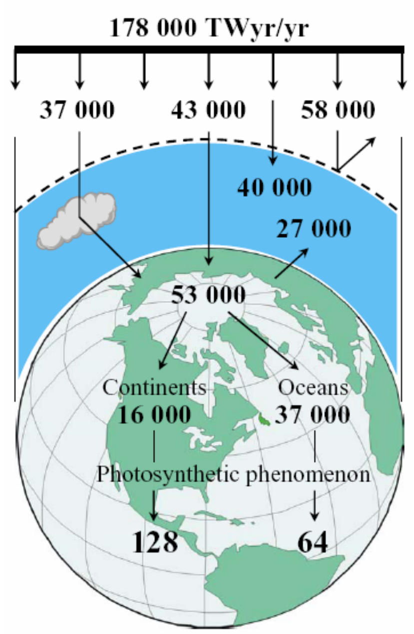


Figure 3: Energy balance repartition for biomass resources from photosynthesis (LASEN, 2003)

All organic material produced by living organisms is called biomass. For fuel, energy and material purposes, wood is one of the main biomass feedstock for humans. Biomass can also be produced by dedicated cultivation for the purpose of energy production. For this application, obviously, only fast growing plants, which give a high yield per hectare, are considered. Miscanthus, sweet sorghum or willows are some examples. After harvesting, growing of the same species or similar plants is necessary therefore leading to biodiversity issues. Moreover, biomass waste streams are often co-products from agriculture and used for energy purposes. Since the main product of agriculture is food, for ethical reasons, biomass for energy or materials production should not compete or interfere negatively with food production.

Waste from household and industry can also be considered as potential feedstock. Wood waste and residues constitute also an important source of directly available biomass. Examples consist of:

- sawdust
- wood chips
- wood waste: pallets, crate discards, wood yard trimming…

Agricultural residues examples are:

- corn residues
- rice hulls
- sugarcane bagasse

- animal waste

At an E.U level some studies have been performed to identify the biomass potential and the potential seems promising (see Nikolaou, 2003).

The global annual 128 TWyr terrestrial biomass potential is partly used by humans. 2% for food, 2% for biomass energy, 10 % for furniture, paper and construction (LASEN, 2003). While 50% of those 128 TWyr are for autotrophic respiration/upkeep of soil quality, the remaining 46 TWyr potential is still interesting and relatively untapped. For actual biopolymer from corn (like polylactic acid a.k.a PLA, which represents 40% of worldwide bioplastic capacity) there is maybe competition between corn based ethanol production or other processes.

At a global level, one can notice that oceanic biomass is not negligible (64 TWyr/yr, see figure 3) and that moreover it is absolutely not used today (a negligible amount is used for food and cosmetics), thus offering a huge potential for future maritime biomass based projects.

2.2 Conventional plastics production

2.2.1 Material and energy flow for fossil fuel based polyolefin production

Polyolefins - which constitute most of the plastics produced today - material and energy flows are depicted in the generic following process chart for polyethylene production (see figure 4). It is important to know that when doing a comparative LCA between bioplastics and conventional plastics, a good knowledge of actual plastic production is necessary. Moreover, the same level of details and information should be reached for both assessment of plastics and bioplastics. Identifying relevant material and energy flows for plastic production (see figure 4) helps us in this task.

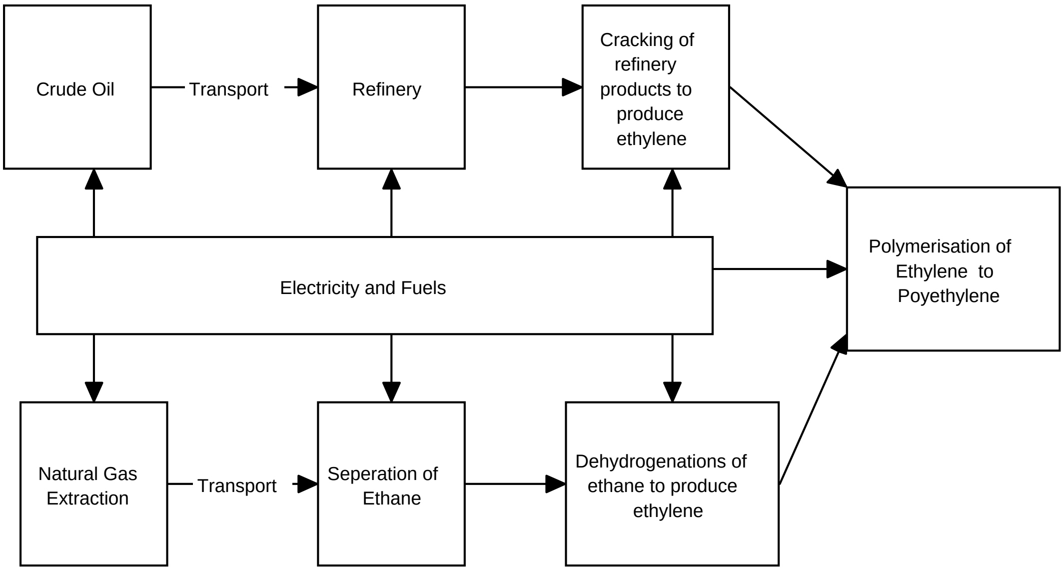


Figure 4: PE routes from fossil fuels (Boustead, 2003)

One should notice that plastics do not come necessarily from oil; feedstock for ethylene and propylene vary a lot around the globe. For instance in the US, propylene comes primarily from Natural Gas Liquids (NGLs are basically ethane and propane) and 60-70% of all plastics are derived from NGL there. A good evaluation of plastics should take this into account – or at least mention a restriction to one specific feedstock composition – and the future bioplastic assessments should also take this criterion into account since, like fossil fuels, biomass composition varies a lot and that with gasification processes for biomass-to-chemicals (BTX) plants, the flexibility of input is quite big.

A summary of major energy, material and emission indicators per kg of ethylene produced is showed in the following table; variations exists depending on the feedstock and data assumptions (see table1), such as electricity sources.

Table 1: Compilation of feedstock inputs, energy data and emissions per kg of ethylene produced from several environmental assessments.

Parameter	**Unit**	**Bou stead (1997)**	**Tellus (1992)**	**IVAM (1996)**	**Tillman (1991)**	**Buwal (1990)**	**Simapro (1994)**	**Pems (1998)**
Oil feedstock	Kg	0.74	0.31	1.42	1.34	0.73	1.40	1.40
Gas feedstock	Kg	0.62	0.66	0.03	0.00	0.75	0.00	0.14
Total Energy	MJ	69.47	68.62	64.25	61.76	67.22	65.63	72.50
CO_2	Kg	0.52	Ns	1.15	1.07	1.32	1.50	1.89
SOx	Kg	0.004	0.0006	0.0062	0.0070	0.0040	0.0023	0.0073
Cx Hy	Kg	0.007	0.00003	0.0053	0.0044	0.0070	0.0046	0.0029
NOx	Kg	0.0060	0.00011	0.0042	0.0022	0.0060	0.0028	0.0051

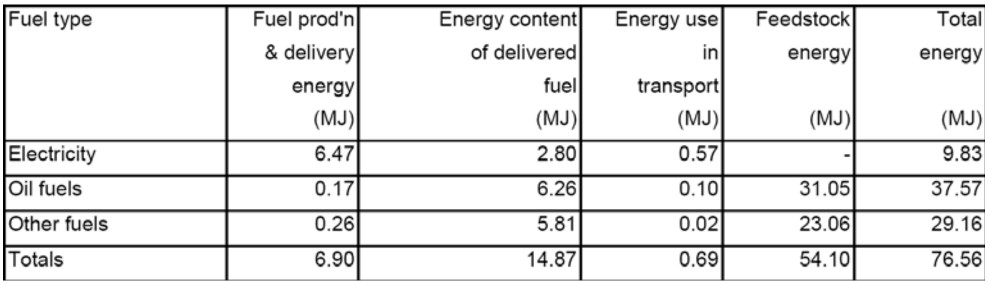
Depending on the geographical region, relevance of material flows could vary. Indeed, sulphur oxides, hydrocarbons and nitrogen oxide emissions vary with the type of feedstock (see table 1). For instance, most of polyolefins in Sweden come from North Sea crude oil whereas most in the US come from liquid natural gas, which is much cleaner.

2.2.2 Description of the magnitude of material and energy flows associated with the conventional plastic production. Identification of the critical ones

It is important for many studies and sustainability assessment for polymers and polyolefins to identify and assess the magnitude of energy and material flows (see table 2 and 3). Indeed, for instance, 4% of the total US energy sources are used for plastics (Comstock et al 2004)

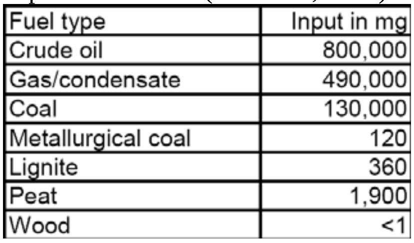
As mentioned above, one can notice the geographical differences between feedstock (see 2.2.1) and the fact that some studies focus on a global perspective thus mixing different data sources from plants around the globe (see Boustead 2003).

Table 2: gross energy required to produce 1 kg of high density polyethylene (HDPE) (Boustead, 2003)



Fuel type	Fuel prod'n & delivery energy (MJ)	Energy content of delivered fuel (MJ)	Energy use in transport (MJ)	Feedstock energy (MJ)	Total energy (MJ)
Electricity	6.47	2.80	0.57	-	9.83
Oil fuels	0.17	6.26	0.10	31.05	37.57
Other fuels	0.26	5.81	0.02	23.06	29.16
Totals	6.90	14.87	0.69	54.10	76.56

Table 3: gross primary fuels used to produce 1 kg of high density polyethylene (HDPE) expressed as mass (Boustead, 2003)



Fuel type	Input in mg
Crude oil	800,000
Gas/condensate	490,000
Coal	130,000
Metallurgical coal	120
Lignite	360
Peat	1,900
Wood	<1

From the PlasticsEurope tables above (Table 2 and 3), we can identify the critical flows which are the fossil fuel flows; whereas the electricity is of secondary importance. This is not the case with bioplastics and will be investigated here after.

2.3 Bioplastics production issues

2.3.1 Available manufacturing technologies for the conventional plastics and the emergent bioplastics

For polyolefins, there are many production processes available: high pressure, solution/slurry polymerisation, gas phase, slurry, bulk loop, etc. Those are state of the art manufacturing technologies (Paulik, 2005).

For bioplastics, many reports have been published about how to produce polymers from biomass (Wondu Holdings, 2004). We will not make another listing of production technologies but will divide them into 2 different categories. We will divide the different manufacturing technologies into two types of routes using the American National Renewable Energy Lab (NREL) distinction between the “sugar” platform (or more generally using biotechnologies; “cold” processes) and the thermochemical platform (“hot” processes) for their Biorefinery concept (see figure 5).

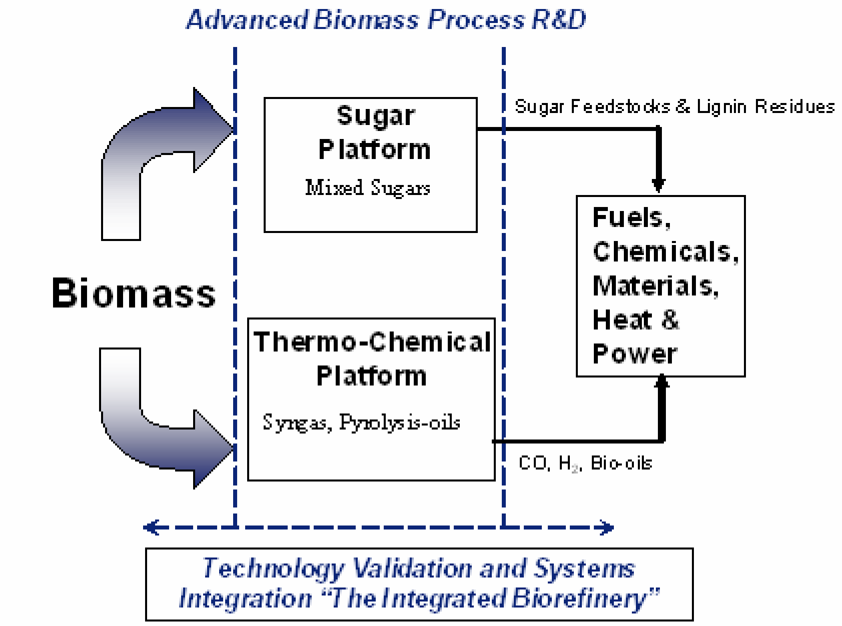


Figure 5: Sugar and thermo-chemical platform concepts (Bain 2004)

As far as we know, even if a lot of research is going on to be able to transform cellulosic biomass directly into sugar and ferment it (see Figure 6), most of today's bioplastics are manufactured using the sugar route from sugar rich sources (via bioengineering equivalent), like for polylactic acid (PLA) production (cf. Figure 6).

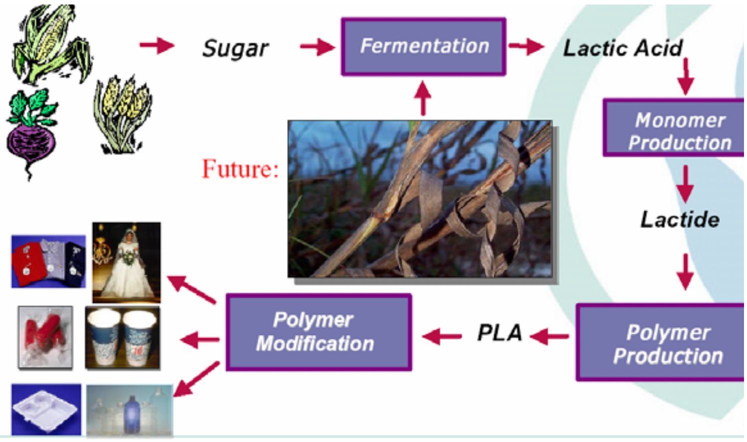


Figure 6: White biotechnologies PLA route (Natureworks llc, 2004)

Some bioplastics could even be produced trough both concept of sugar platform and thermochemical platform (see figure 7). It is then only a strategy choice depending on the feedstock availability and cost of material since the biotechnology route could be more efficient (see figure 7), or not.

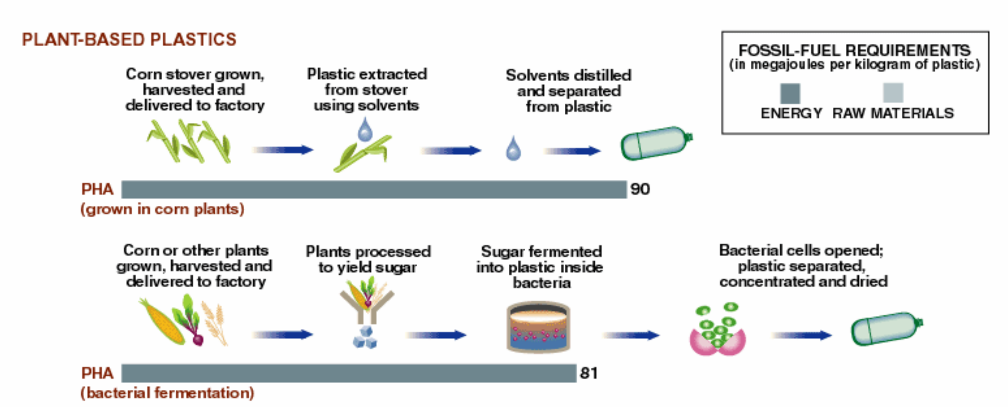


Figure 7: 2 processing routes for PHA production (Comstock et al, 2004)

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Many reports and research papers are available regarding the sugar platform and the environmental potential of those processes (Natureworks llc, 2004). The bioengineering platform based polymers are driven by the need of specific new functionalities of polymers like biodegradability or compostability and most of the research focuses on biodegradable/compostable[7] biopolymers (European Bioplastics, a.k.a IBAW, 2005).

Today, most available manufacturing processes for production of bioplastics are based on the sugar platform whereas the existing thermochemical platforms (see Choren GmbH, MHI ltd) stop at the production of biofuel. However it is possible to go further downstream and to make polymers like polyolefins out of biomass (see routes described in figure 8), but those processes remain relatively unexplored in terms of environmental potential. It is one of the reasons why we are going to go further in the modeling of this specific route in sections 3 and 4.

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[7] We kindly remind the reader to remember the exact meaning of the words biodegradability and compostability. If waste management systems capacity is exceeded, or if littered in the environment, only (bio)degradable plastics will effectively degrade. PLA for instance, will not. Moreover, the term biodegradable or compostable could be applied to any material whether it is from bio origin or not. This means that fossil fuel based degradable plastics could be part of the solution for plastic littering issues. However this has not been studied since it is out of the scope of our study.

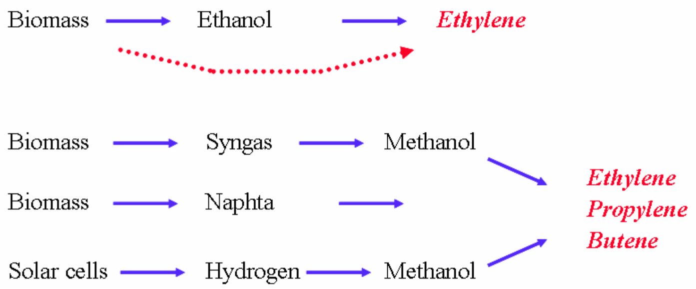

Figure 8: Light olefins routes (Hjertberg, 2005)

The main potential processes identified to produce bioplastics via the thermochemical platform are:

- Ethylene/propylene from methanol-to-olefins (MTO) processes via methanol or dimethyl ether (DME) from bio-syngas
- Ethylene/propylene from naphtha cracking via naphtha from biomass (by product of Fischer Tropsch FT synfuel for instance)
- Ethylene from ethanol dehydration via ethanol from biomass.[8]

There may be other routes, but we will first stop at this screening which seems representative of the available manufacturing technologies. Indeed, even if the full train from biomass to polyethylene/polypropylene via syngas does not exist, each step is technically feasible and has been implemented at least on a laboratory scale (see section 3.1). Indeed, for most of the steps described here, a pilot or an industrial unit already exist (Nouri & Tillman, 2005).

2.3.2 Description of the magnitude of material and energy flows associated with the biopolymers

To position the biopolymer studies, one must have an idea of the magnitude of material and energy flows with the same level of understanding – if possible – as with the conventional polymers. Existing studies are available about some production routes of biopolymers such as polylactic acid (PLA), Polyhydroxyalkanoates (PHAs), etc.

For PLA, 2.5 kg of corn is needed to produce 1kg of PLA (Natureworks llc, 2005) and so 350 000 ton of corn are needed annually for the 140 000 ton plant from NatureWorks llc in Nebraska. The energy use for producing 1kg of PLA is 25% less fossil energy than high density polyethylene a.k.a HDPE. No transport of environmentally hazardous material, like oil, etc.. , occurs during biopolymers production, decreasing the risk of spillage and pollution.

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[8] It can be worthy to produce ethanol from ethylene, or vice versa in some regions (see appendix 2)

For the Biomass to polymer thermochemical route via syngas and methanol concept (see figure 8 above), about 11 kg of biomass (wood waste) are required per kg of polymer, and about 70 MJ primary energy is needed.

2.4 Performance issues

2.4.1 Technical performance characteristics of the current plastics and emerging biopolymers

The technical performance of bioplastics should - for marketing reasons, even if further discussion about this could be investigated - at least be the same than their fossil based counterparts. The available and upcoming processes to produce bioplastics achieve this criterion (cf. Figure 9 and table 4).

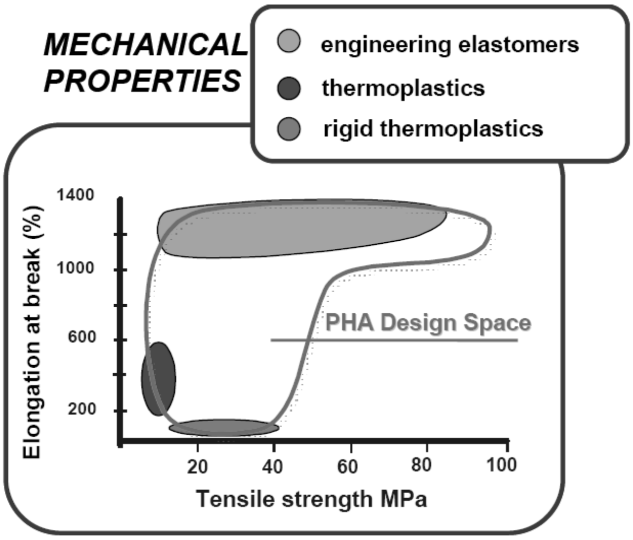


Figure 9: Polyhydroxyalkanoate (PHA) design space (Metabolix, 2006)

Table 4: comparison of PLA and polyethylene (low density and high density: LDPE and HDPE) properties (Bixler et al, 2005)

	PLA	LDPE	HDPE
Glass Transition T (^{o}C)	55-70	-40	-120
Melting T (^{o}C)	130-215	98-120	127-135
Ceiling T (^{o}C)	>500	~400	~400

Crystallinity (%)	10-40	50-70	80-95
Yield Strength (MPa)	49	4.1-16	21-38
Tensile Modulus (GPa)	3.2	0.1-0.26	0.41-1.24

For most application, biopolymers are ready in terms of technology to be used in the same applications than classic fossil based polymers.

For most of the new biopolymers produced, few technical limitations exist that could stop the transition towards biobased plastics. For instance PLA can today be processed easily in polyethylene terephthalate (a.k.a PET) extrusion machines without any big changes (NatureWorks 2005). However it cannot be microwaved, which in some case could be a flaw. For the example of polyolefins from biomass via syngas processes, the bioplastics obtained have the same properties than the fossil based ones.

2.5 *Market issues*

2.5.1 Description of current plastic usage trend

Diverse applications exist from building to packaging (see pie chart). The trend for plastic is to penetrate new markets and replace other materials like glass, paper, metals, etc.

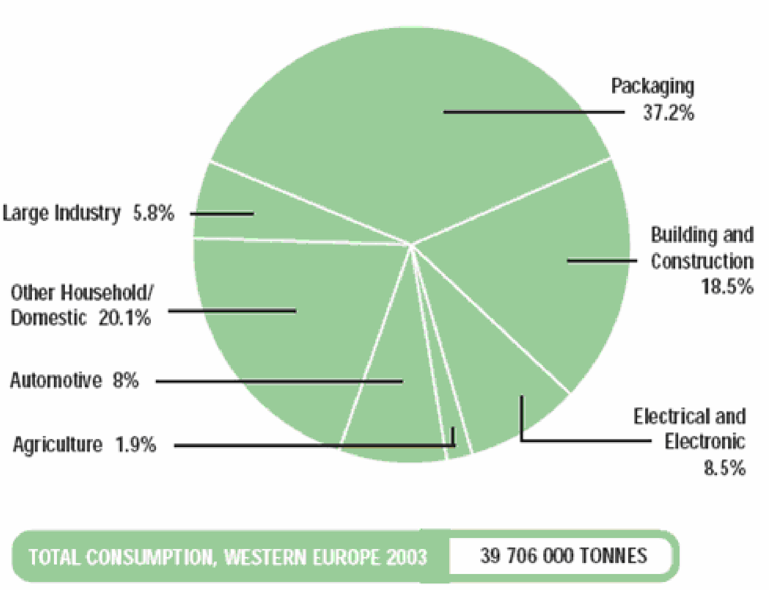


Figure 10: Plastics consumption by industry sector in Western Europe in 2003 (PlasticsEurope 2003)

2.5.2 Focal market and application for the biopolymers

The applications for bioplastics are numerous and can be divided into 2 categories:

- Small scale production, high cost (medical implants, high tech applications)
- Large scale production, low cost (packaging, hygiene applications…)

We will first focus on packaging applications since it is in mass the biggest use and thus has a great environmental impact.

2.5.3 Current level of demand (current and emerging)

"… in the next ten years the world consumption of plastics will grow faster than the gross domestic products of all regions. Plastics are the materials of the 21st century. For the entire world we are expecting growth of over five percent per year…" (Feldmann, BASF 2001).

"Demand for plastics remained strong across all industry sectors in 2002 and 2003, although actual growth was limited, reflecting an overall downturn in the world's economy. Although the majority of sectors showed no significant increase in consumption compared to 2002, the automotive sector did show significant growth, increasing by 5.7 per cent in 2003. The packaging sector continues to be the major consumer of plastics. However, with the share of packaging in total plastics consumption remaining stable at just over 37 per cent in 2002 and 2003. Across other industry sectors there was relatively little change. The building and construction sector remains the third largest user of plastics, with a 2 per cent increase in consumption in 2003. The agriculture sector consumed the same 1.9 per cent of plastics in both 2002 and 2003". (PlasticsEurope 2003)

As pinpointed above by representatives of the sector, the current demand for plastics is important and steady thus creating a potential substitution market for bioplastics. Morever new regulations (like the recent Danish packaging law on packaging or updated EU directives, cf. Directive 2004/12/EC of the European Parliament and of the Council of 11 February 2004, amending Directive 94/62/EC on packaging and packaging waste) and specific properties of biopolymers (like compostability or biodegradability) could increase the penetration rate of bioplastics.

Moreover the future seems quite bright. Indeed, Kozaburo Tsukishima, general manager of Toyota's biotechnology and afforestation division, says bioplastics *"could really explode as a business, and may have the biggest growth potential out of all of our operations…//…one-fifth of the world's plastic would be bioplastic, equivalent to 30 million tonnes. We want to be supplying 20 million tonnes of bioplastics by 2020, which would amount to about four trillion yen in revenues if we sold it at 200 yen per kilogram"*

Market for bioplastics is growing, as estimated by IBAW, pan-European consumption of bioplastics in 2003 was at 40,000 tons; this indicates that consumption has doubled from 2001.

However the penetration rate remains today insignificant…less than 1% of total polymers…even if a tendency due to oil/biomass price ratio increase is boosting the bioplastics all around the world (with a good advance for PLA and NatureWorks llc).

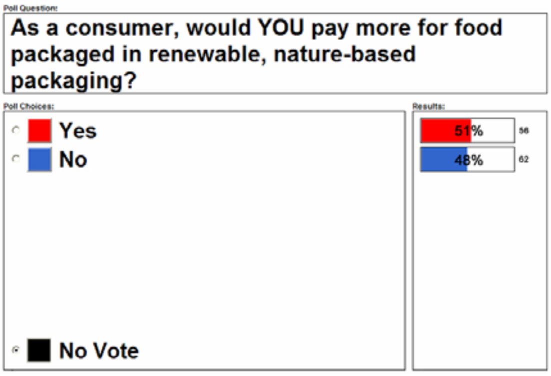
2.5.4 Current state of early stage biopolymer selection in industry

To have an idea of the state of biopolymer selection in industries, one can take a look at what are the biopolymers produced nowadays in the biggest amount. Except Brazil and its allegedly 1 million ton/year polyethylene produced from ethanol (Klass, 1998); while there are an estimated 47 producers of bioplastics worldwide, only two have a capacity greater than 40,000 tonnes/year and six greater than 10,000 t/y. The NatureWorks PLA plant in Nebraska has a capacity of 140,000 t/y and represents about 40% of the world capacity (NatureWorks llc, 2005).

From a general point of view it seems that the current early stage situation is in favour of PLA. Even for specific applications other than packaging, PLA seems appropriate and can rule part of those niche markets (ie. PLA for surgical implants, PURAC 2006).

2.5.5 Measuring the market's/customer's value for the technical, economic and environmental characteristics of the current plastics and how they make trade-offs among those characteristics

Plastic as packaging and its possible bioplastic counterparts, has been studied from a market's/customer point of view. From a strict consumer point of view, the answer about spending more for renewable packaging is interesting (see poll figure 11).



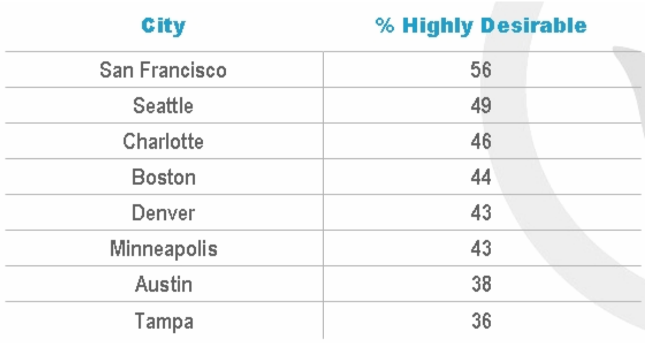
As a consumer, would YOU pay more for food packaged in renewable, nature-based packaging?

Figure 11: Half of the consumers will pay more for renewable packaged food products (Natureworks llc, 2004)

The consumer is clearly making tradeoffs when buying bioplastics. About this, a very interesting survey has been conducted by Grapentine Inc for NatureWorks llc and the PLA plastic. The main conclusion is that nature based packaging is an excellent booster for natural products sales (natural-in-natural trend).

Among the conclusions from this study is the customer’s interest for biopolymers (PLA is presented as a 100% corn based plastic that can be composted) and the consequently substantial segment of 41% of respondent which find the concept desirable, compared to two other concepts used for index: fresh packaged spices/herbs (48%) and organic meat and vegetables (29%). What is also interesting is the geographical distribution of the market’s/customer’s value for the biopolymer among the US (see table 5).

Table 5: Bioplastic concept desirability through the US.



City	% Highly Desirable
San Francisco	56
Seattle	49
Charlotte	46
Boston	44
Denver	43
Minneapolis	43
Austin	38
Tampa	36

The results show that the north and west is more attracted to bioplastics than the south. This study shows also how customers make trade off among economic and environmental characteristics (see figure 12).

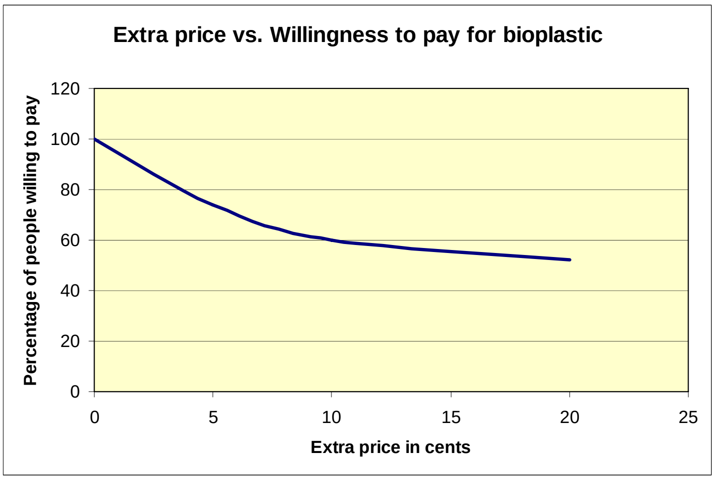


Figure 12: Renewable packaging buying desire decrease with the extra price to pay (NatureWorks llc 2005 adapted).

2.6 Sustainability research issues

Much work has already been done on bioplastic sustainability assessments. Most of them concerns the environmental impact new bioplastics would have on the environment, compared to fossil fuel based plastics.

2.6.1 Biomaterial sustainable assessments: environment, economics and social aspects

To understand and try to improve environmental assessment tools, it is important to know what kind of methods and tools are state of the art. Many sustainability methods and tools are available today. The tools and methods can be divided into the following groups: management tools, like ISO 14001 and EMAS, assessment tools, like Life Cycle Assessment (LCA), communication tools, like Environmental Product declarations (EPD) and other more normative instruments, like legislation and standards.

We have looked mainly at assessment tools like LCA (Baumann & Tillman, 2004), process modeling/integration (Gundersen, 2002) and eco-efficiency (Kicherer, 2005). However, a close contact to other tools like management tools (Erlandsson,

2006) or environmental policies (Sterner, 2002) keep us open to different sustainable strategies where “when and where” to apply assessment tools can vary. It helps us to have more experience in how to build a potential method to improve our assessments regarding our particular case of bioplastics (i.e early design phase for plastic producers).

LCA is one of the most commonly used tools to deal with questions regarding sustainable new materials. LCA literature about bioplastics is abundant (Patel, 2001), (Vink et al, 2002), (Narayan, 2004), (Wolf et al, 2005) and is focused mainly on CO_2 emissions and energy used. In figure 13, an illustration of such LCA literature results is displayed with a number of polymers studied both biobased and conventional.

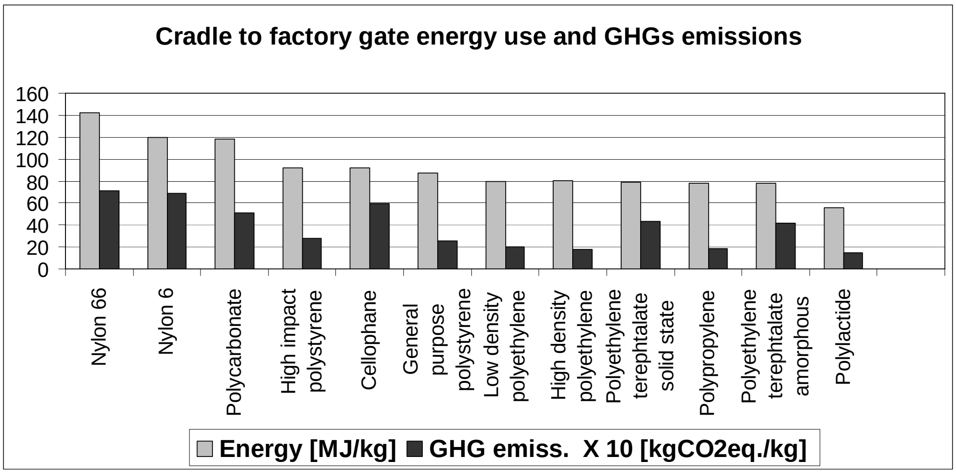


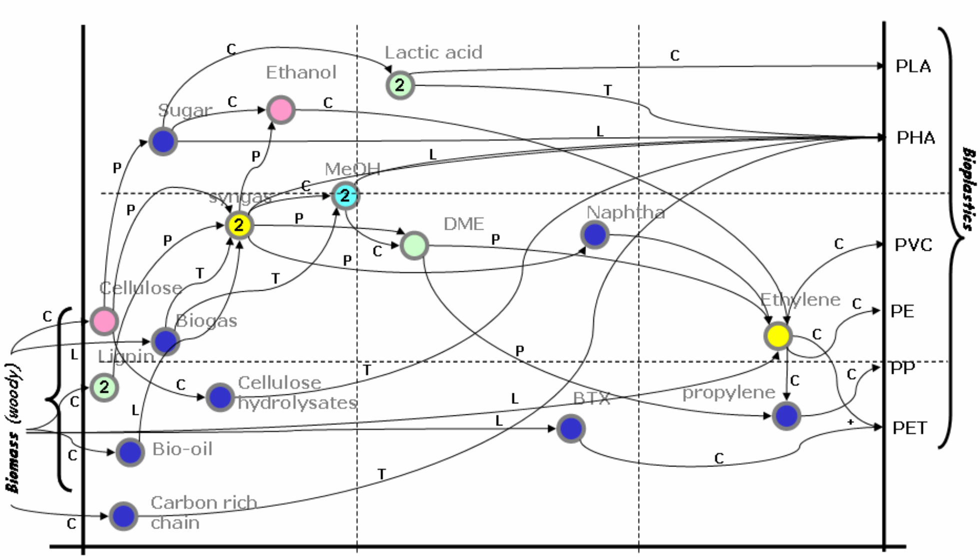
Figure 13: Energy use and GWP potential for different polymers (Vink et al, 2003).

Another aspect of sustainability that has been looked at is economics. There are indeed many ways to assess bioplastics economical performances but they won’t be dealt with here. However by combining LCA thinking with specific tools like cost models or process modeling, (see PBCM, Kirchain and Field, 2000) one could improve the effectiveness of such tools. We will work through a lifecycle perspective and try to include these other cost aspects in an integrated assessment.

Finally about sustainability assessment, one forgets often the social aspects. Their inherent complexity and difficulty to be grasped make social aspects hard to assess or at least to process in the same quantitative manner as environmental or economic issues. However, a simple one like the impact on employment for emerging technologies via the number of new jobs they can create can be relatively easily assessed. We will show in section 4.4 how to calculate the number of jobs created using process modeling data.

3 Bioplastics: the case study

The detailed case study following the above research plan will be now presented. After a first technology screening from the biopolymer background (see 2, Figure 1) where different intermediates from biomass to plastics have been identified as potentially implemented within 20 years (see paper II) using some indicators like technical status or patents numbers (cf. Figure 14), we chose a process towards bioplastics mainly based on thermochemical process units and syngas technologies (see figure 8) as a main object of study. Wood waste as a feedstock is gasified to produce syngas which is then transformed into methanol which is transformed in ethylene and propylene using Methanol To Olefins (MTO) technology and then polyolefins unit to produce biopolyolefins.



Key: T = in theory; L = in labs; P = pilot; C = commercial

Figure 14: Biomass to polymer routes. Colored intermediates are favored by some indicators (see paper II) and form the first pool of routes that will be environmentally assessed.

3.1 Biomass to polymers (BTP) process presentation

As mentioned before, we picked up the BTP [9] process out of a pool of other bioplastic production routes since many drivers seemed favourable (Nouri & Tillman, 2005). This process would convert biomass to clean syngas, then to

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[9] We intentionally use abbreviations close to the natural gas monetization ones like Gas to polymers (GTP) since the BTP process is based on the same concepts than GTP. Indeed, there are many similarities between biomass and natural gas (see appendix 3)

methanol which will be converted to C_2-C_4 olefins, based on existing technology and finally polymerized in polyethylene and polypropylene.

The biomass to plastics route consists basically of 4 steps and a relatively simple flow sheet can be drawn (see figure 15). However due to its inherent sensibility to many drivers - pushes and pulls (Nouri, 2005) - there are many possible variations of this scheme (e.g. alternative feedstock such as plastic waste results in plastics waste to plastics concept a.k.a PTP, developed by Hydro Polymers and studied in more details in section 4.2.2).

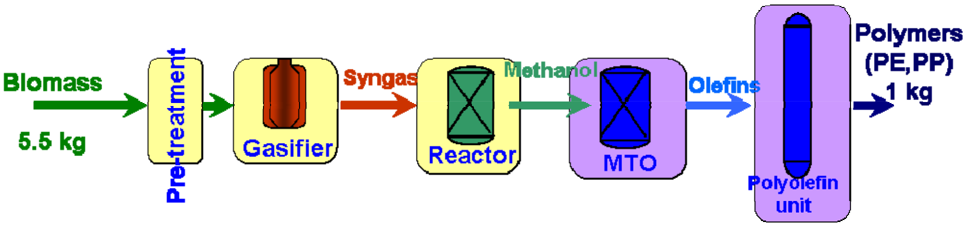


Figure 15: waste to polyolefins process steps with mass balance

We will now go through the different process steps in some detail with respect to what they do and their technical status.

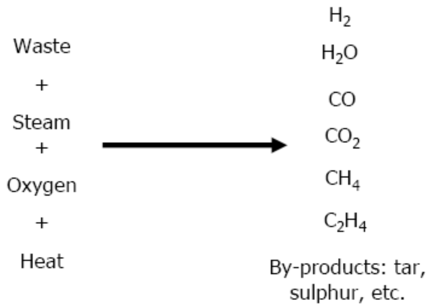
3.1.1 Pretreatment

Before gasification, feedstock has to be pre-treated. This consists mainly in, screening, size reduction and drying. It is an important step since cost of this preparation could be about 5% of the total equipment investment costs (Ekbom et al, 2003). Drying is generally the most important pre-treatment step. It reduces the moisture content to about 10% using steam or flue gas (Ekbom et al, 2003). This pre-treatment step is not necessary for coal or plastic waste gasification. For black liquor, evaporation is already done for combustion in conventional recovery boiler an important pre-treatment step.

3.1.2 Gasification and methanol production

A biomass-to-methanol fuel plant via gasification (or BTL: Biomass To Liquid plant) comprises usually: an air separation unit (ASU), a gasification island (dryer, gasifier…), some gas-cleaning sections and a methanol synthesis.

Conversion of waste/biomass to synthesis gas (H2, CO2 and CO mixture) suitable for methanol synthesis takes place in the gasification unit. Circulating Fluidised bed gasifiers seems promising for forest residues feedstocks and there are existing demonstration projects for chemical production based on this type (Chrisgas project, 2004)



Gasification chemical reaction (1)

The gas at the outlet of the gasification unit (see reaction 1) has to be cleaned before downstream processing. Indeed, the produced syngas contains tars, dust, alkalis, sulphur - biomass inherently contains sulphur in very low proportions, about 0.03 % (Scahill, 2003), that can lead to sulphides formation - and halogens that can poison the catalyst or corrode the different units of the downstream process. Whereas conventional technology can be applied using gas cooling, low temperature filtration and water scrubbing, hot gas cleaning technology is not yet well proven. However due to strong investments and research – partly due to syngas process interests – hot gas cleaning is a very attractive and forthcoming cleaning concept (Hamelinck et al 2001).

Contaminant like tar and methane has also to be removed which may be done with newly developed tar cracking and methane reforming catalysis.

The next step in the concept is the production of methanol from syngas, which is achieved by a conventional methanol process (Liquid Phase methanol reactor). The main reactions are given below (2) and (3), both are exothermic reactions. In order to obtain maximum catalyst activity, 5% of the feed should be CO_2 (Moulijn, 2003).

$$CO + 2H_2 \rightarrow CH_3OH \qquad (2)$$

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O \qquad (3)$$

The conversion in the methanol reactor is low; hence a high recycling rate of the unreacted syngas is necessary. Part of the recycle gas is taken out as a purge gas in order to avoid build up of inert in the system. The purge gas is used as an energy source for steam generation. The methanol process given in Figure 8 differs from plants converting natural gas into methanol, since the following step, the MTO plant tolerates crude methanol as input. This means that the separation of methanol and water in distillation columns is avoided. The technology status of BTL via gasification is at a Process Demonstration Unit (PDU) phase with the main 2 units identified in Freiberg/Saxonia from Choren GmbH in Germany (FT-diesel production) and in Kawagoe from MHI ltd in Japan (Methanol production).

3.1.3 Methanol/DME to Olefins

In the MTO process methanol is converted to olefins (mainly ethylene and propylene) over a catalyst. The principal reaction is given as Equation 4:

$$5CH_3OH \rightarrow CH_2CH_2 + CH_2CHCH_3 + 5H_2O \qquad (4)$$

For a methanol to olefin unit, about 3 tons of methanol are needed to produce 1 ton of light olefins with equal amount of propylene and ethylene. The technology which is at a demonstration plant status and ready for commercialization is mainly two types:

- Methanol/DME To Propylene with MTP and DTP pilots from Lurgi GmbH and JGC Corp, respectively, that produce mainly propylene and some other by-products.
- Methanol to Olefins (MTO) with UOP/Hydro and ExxonMobil process demonstration units (PDU) producing both ethylene and propylene with a ethylene/propylene ratio that can be changed from 0.75 to 1.5 (UOP/Hydro data). ExxonMobil PDU C2/C3 ratio is 1.

3.1.4 Polyolefins production

The ethylene and propylene are then polymerized to polyethylene and polypropylene using polyolefin units like Borstar units commercially available from Borealis.

Moreover, polyolefin additives compatible with the existing polyolefin units are available on the market to add specific properties like controllable degradability. Indeed, our meeting with Nor-X industries AS managers in Norway concluded that it is completely possible to add Nor-X degradable additives in the BTP concept to create bioplastics that can degrade automatically in the environment[10] if littered. The production of Nor-X degradable additives as well as its impact on the environment when degradation occurs has not been assessed due to insufficient time, but discussions with researchers at Sintef (Männle, 2005) and Nor-X AS (Rødseth, 2005) concluded that the added environmental burden should be

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[10] “Nor-X Degradable are additives that are tailor-made to degrade plastic products made of LDPE, HDPE and PP. The degradation process starts when the products are influenced by UV-beams (sun light) and/or excessive heat (land fills). The degradation time can be tailor-made according to customer’s individual needs. Additives from Nor-X Industry AS do not contain materials that harm the environment in any way. When recycling occurs with Degradable plastic, Nor-X Industry AS, SINTEF and Emballasjeretur have made a test that shows that plastics containing Nor-X Degradable does not harm the recycle process. Quite the opposite, there are signs that shows that additives from Nor-X Industry improves the quality of recycled plastic”. From Nor-X Industry AS www.nor-x.no

negligible compared to the total impact during the BTP route. These degradable additives are crucial if the BTP route is targeting the biodegradable bioplastic applications. The first information and contacts regarding those additives seems conclusive, but more research has to be done to draw a clear conclusion regarding the total environmental impact and cost of those additives.

3.2 Stream-lined LCA of BTP process

As described in 3 in Figure 1, a first basic environmental assessment of the BTP process will be performed in the form of an LCA. First GHGs emissions and then the energy use will be accounted from a cradle to gate perspective

The general flow sheet assessed will look like the one in figure 16:

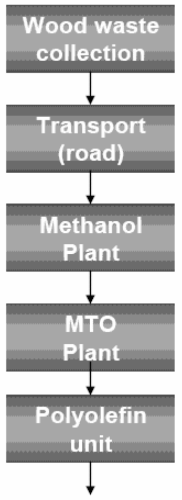


Figure 16: flow chart for the BTP route from cradle to gate base case

We will now account the green house gas emissions for the BTP route. The CO2 figures represent the actual emissions occurring during each process. When CO2 emissions stem from biomass, only the net emissions are counted, i.e. CO2 of biomass origin is not accounted for.

The total net GHG emissions for the BTP route are 267 g CO2eq/kg for a Cradle-To-Gate (CTG) and worst case scenario cf. table 6.

Table 6 Net GHGs Emissions for polymer via BTP route (Nouri & Tillman, 2005)

Collection, chipping and transport	84
Gasification + methanol (MeOH)	12

synthesis	
MTO	107
Polyolefin unit	64.3
Total net CTG GHGs emissions	**267 g CO2eq/kg**

Bio-based polymers and particularly polymers from the BTP route seem to offer important environmental benefits regarding GHG emissions.

The energy use of the BTP process is distributed as follow:

From a cradle-to-factory gate perspective, the total primary energy consumed for the BTP is 3.6 + 0.6 + 57.6 + 2.25 + 6.12 = **70.2 MJ/kg** of polymer produced (cf. table 7). Assuming that 85% of the electricity is from non renewable sources (EDWARDS 2003) the non renewable energy use of the BTP process is thus 3.6 + 0.6 + 57.6x85% + 0.14x85% + 1.33 + 2.1x85% + 0.11 = **56.5 MJ** per kg of HDPE is non renewable energy.

Table 7: Total primary energy consumed for polymer production via the BTP route (Nouri & Tillman, 2005)

Collection, chipping and transport	3.6 + 0.6
Gasification + MeOH synthesis	57.6
MTO	2.25
Polyolefin unit	6.12
Total primary energy consumed	**70.2 MJ/kg of polymer**

The total energy consumption to produce 1kg of polymer is divided into: 8.2 MJ electricity which with a 35% efficiency gives a total primary energy associated to electricity of about 23.6 MJ of which 85% i.e. 24.4 MJ are considered non renewable; 6.2 MJ fossil energy and about 115 MJ of biomass are also required.

A summary of the positioning of the BTP route as the most environmentally friendly compared to existing polymers routes can be seen in the following figure 17:

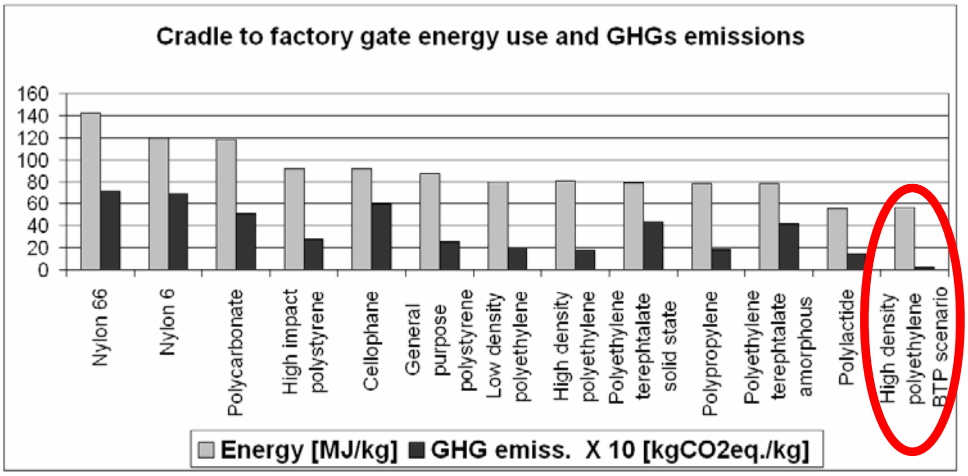


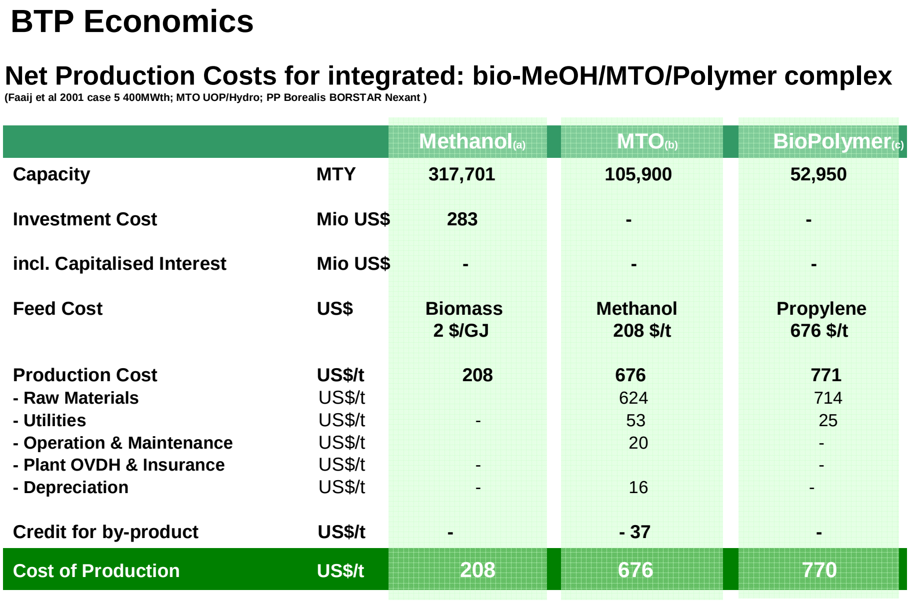
Figure 17: positioning of the BTP route using GWP and energy use from a cradle to gate perspective.

For all calculation details see appendix 4.

3.3 Cost of Biomass to polymers process

As displayed as 4 in Figure 1, following the environmental assessment of the BTP route is a cost analysis of plastic production via the BTP. The cost of production of biopolymer via the BTP route could be estimated by compiling and extrapolating financial data available from the main studies performed for biomass to methanol production routes and the major MTO concept designers (UOP/Hydro and Lurgi with its MTP). This leads to a cost of production for bio-polypropylene of about 770 $/ton cf. table 8.

Table 8: Cost of production estimation for bio-polypropylene (Nouri & Tillman, 2005)



BTP Economics

Net Production Costs for integrated: bio-MeOH/MTO/Polymer complex

(Faaij et al 2001 case 5 400MWth; MTO UOP/Hydro; PP Borealis BORSTAR Nexant)

		Methanol(a)	MTO(b)	BioPolymer(c)
Capacity	**MTY**	**317,701**	**105,900**	**52,950**
Investment Cost	**Mio US$**	**283**	**-**	**-**
incl. Capitalised Interest	**Mio US$**	**-**	**-**	**-**
Feed Cost	**US$**	**Biomass 2 $/GJ**	**Methanol 208 $/t**	**Propylene 676 $/t**
Production Cost	**US$/t**	**208**	**676**	**771**
- Raw Materials	US$/t		624	714
- Utilities	US$/t	-	53	25
- Operation & Maintenance	US$/t		20	-
- Plant OVDH & Insurance	US$/t	-		-
- Depreciation	US$/t	-	16	-
Credit for by-product	**US$/t**	**-**	**- 37**	**-**
Cost of Production	**US$/t**	**208**	**676**	**770**

(a) Production cost of methanol from biomass using data from methanol production concept 5 (Carlo N. Hamelinck, A. P. C. F.2001)
(b) production cost of propylene from methanol using MTO technology (Andersen et al 2003) assuming methanol feeding price at 208 $/ton.
(c) Polypropylene unit economics (Lurgi Oel Gas Chemie 2002) assuming propylene feeding price at 676$/ton.

With US prices of about 1600 $/ton for polypropylene (ICIS March, 2006), the first cost estimation seem to show a potential for viability for the BTP route.

This 770 $/ton can be compared with the 1006 $/t cost of production (Nexant, 2006) for non renewable polypropylene. We use the same presentation and calculation approach than with the gas to propylene concept presented for instance by Lurgi (Lurgi 2003).

Capital Expenditure (CAPEX) is also a crucial number: knowing how much is going to cost to build a biopolymer plant is the first step towards cost analysis and investors networking (i.e. it cost more than 7 billions dollars to build a GTL plant in Qatar, leading to very complex joint ventures between major oil companies; the same JV models could be applied for expensive biorefineries). Total investments are about 265 MM$(2003) for the bio-methanol plant (548 tonMeOH/day, 53,000 MTY polyolefin), 720 ECU1994 per ton ethylene capacity (Joosten 1998) for the MTO and 39 $(2001) fixed cost per ton polyethylene produced for the HDPE unit respectively.

The cost of production decreases with the production volume and the model used is a classic economic one with some different foreseeable cost reductions like cheap biomass, technology learning and large scale (see Hamelinck et al, 2001, p 20, 58). For our BTP process an illustration of this phenomenon is given in figure 18 here after:

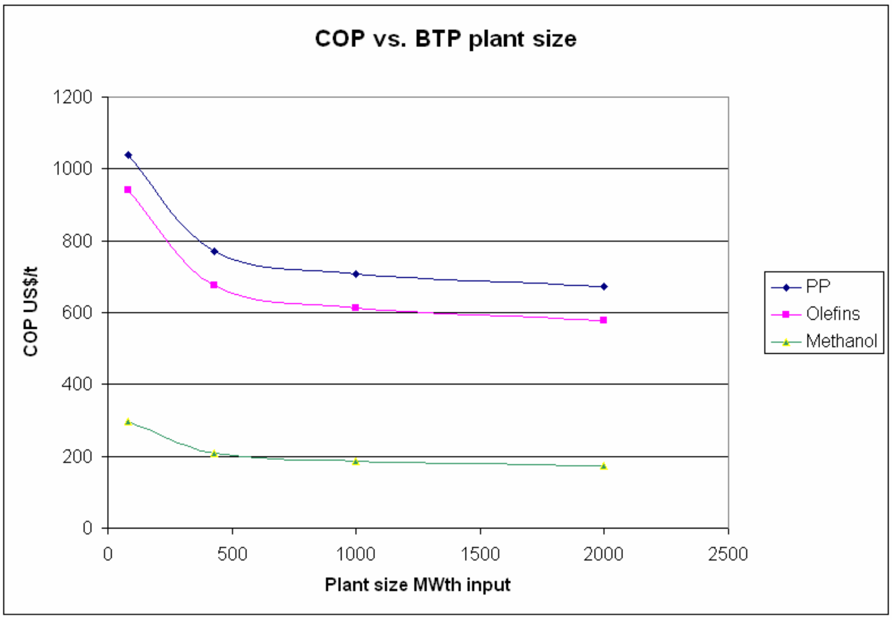


Figure 18: Cost of production of methanol, olefins and polypropylene from biomass vs. the size of the plant.

Results seem encouraging for the BTP route but need to be qualified and compared to other bioplastics.

It could also be interesting to see what are the values of the products along the biomass monetization process. The value of the products from 1 ton of biomass dry substance depending on how far the biomass monetization process is conducted is shown in Figure 19.

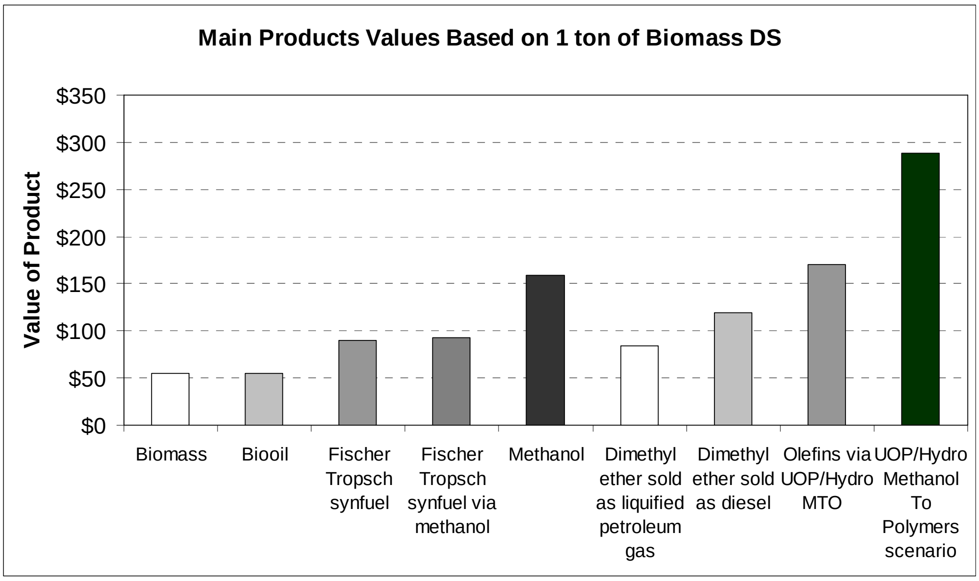


Figure 19: Biomass monetization products values

4 Process modeling and assessments

As mentioned in 5, figure 1, we will now present the combination of a process modelling with environmental and cost assessments. Let us begin with the combination of LCA and process modeling.

4.1 Present situation

Today, LCA is the main tool for assessing environmental performance of bioplastics and emerging technologies for bioproducts as described in (2.2.1). For bioplastics, most of the environmental assessments are following technology screenings of production routes. As mentioned in paper II, the use of technology screening information uncritically for environmental assessment prove to be dangerous. Thus LCA of bioplastics are often incomplete (some even presenting only one waste management option for plastics designed to fit multiple waste management systems, like composting, recycling, etc.)[11] or simply out of scope (see paper II). Moreover even with LCA and dominance analysis it is often impossible to know exactly where are the emissions formed and thus hard to make accurate futuristic scenarios regarding potential environmental improvement (change in the electric system, logistics, etc.). Therefore process modeling can be of great help.

4.2 Process modeling and LCA

Using process modeling for improving the quality of environmental assessment and LCAs for instance has been very conclusive. Indeed, process modeling softwares – like HYSYS that we will use - are tools for managers and engineers to find the optimum process design and link business objectives with process design. They allow simulation of different process designs, specification of process equipment, evaluation of the effects of changes (feed, equipment etc) on the process and the assessment of process deficiencies. They also offer modules where the financial outcome of the process may be projected (AspenTech, 2006). Environmental issues, however, are assessed by these softwares only in a very limited way. Energy use and other resource consumption such as feed-stock are modeled, but they do not allow for modeling of emissions to the environment, and hence not environmental impact. They do thus not support modeling of what-if scenarios with

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[11] It is crucial to understand the flaws of these kinds of LCAs such as the one presented by Patel (2001). When producing degradable plastics, one adds value to a material by allowing it to fit in more than one waste management system , like composting and recycling. The arguments of some authors to present only scenarios with incineration of bioplastics because it is most likely what would happen if they are introduced in EU (since incineration is quite dominant there) is very wrong. To make it clear, it would be like presenting the well-to-wheel study results of a flexifuel vehicle running only on gasoline, because it is most likely what would happen if they are introduced in a market where gasoline is dominant and alternative fuels for flexifuel are not available. Moreover, the incompleteness of those LCAs, considering only incineration for degradable plastics, leads directly to fallacious promotion leaflets like the one from Plastics Europe in section 2.1.1

respect to environmental aspects. LCA-process modeling combination could fill this gap and the way to achieve this has been developed and used during this project. The combination of process modeling and LCA helped to have a better understanding of the hot spot of the process and a much precise dominance analysis.

4.2.1 Principle

Since most of the environmental impact of new technologies/products is “locked in” by decisions made in the early-design phase (Godoy et al, 2003), combining LCA and process modeling to assess the impact of different scenarios in the early design phase can help reducing the total environmental impact of a project (see Figure 20). Integrating LCA and process modeling, enables engineers to reduce the risk of ignoring environmental constraints during the ideation phase which is the phase indeed when they are the most vulnerable regarding environmental impact (tendency to work “freely” and great-effect decisions).

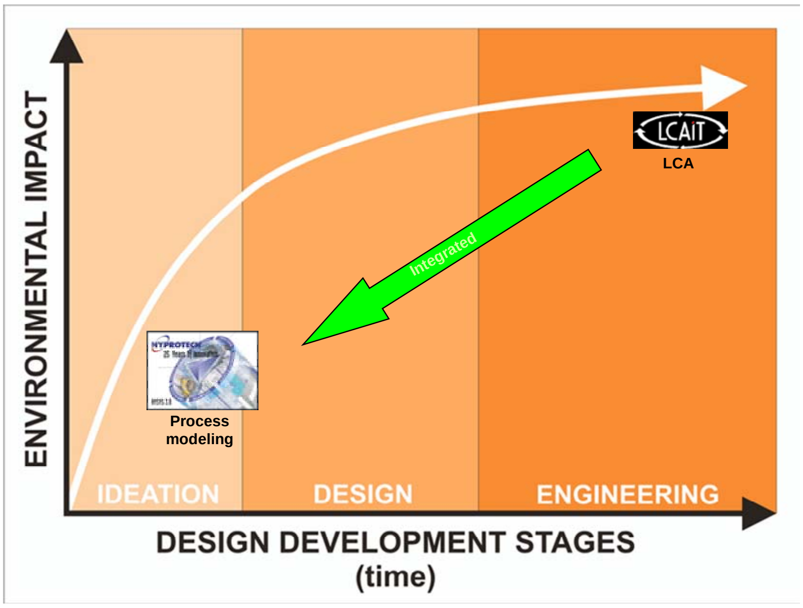


Figure 20: LCA-process modeling integration in early design phase (Godoy et al, modified 2003)

4.2.2 Example

We are now going to present an example where a combination of LCA and HYSYS model was done for the biomass to plastic (BTP) route and the plastic waste to plastics (PTP) one.

Gasification models are complex. For both simplicity and practical reasons, the gasification step was not included in the HYSYS process model. Instead, data was taken from the literature. For the subsequent steps, a HYSYS model was built based on industrial data (Step 1, Figure 21). The model takes the raw syngas from the gasifier as an input and treats it all the way to methanol. The steps in the HYSYS model were the following (Figure 21):

- Water removal from the syngas, done by component splitter.
- Water gas shift (WGS) as a two-stage process, with addition of water to obtain a H_2/CO-ratio of 2 after the WGS.
- Removal of sulphur done by a component splitter using the same split fraction for all scenarios.
- Removal of CO_2 by two component splitters, where the first one is “recycle gas” to the biomass gasifier, and the second is “flue gas.” For plastic waste, the outputs from the first and second splitter are classified as “flue gas” since no recycle gas is needed in the gasifier.
- Reaction of cleaned syngas to methanol (methanol synthesis), at a conversion rate of 92%. The reactor is followed by a component split of methanol, water and non-reacted syngas. The unreacted syngas is used as fuel gas in the steam island.

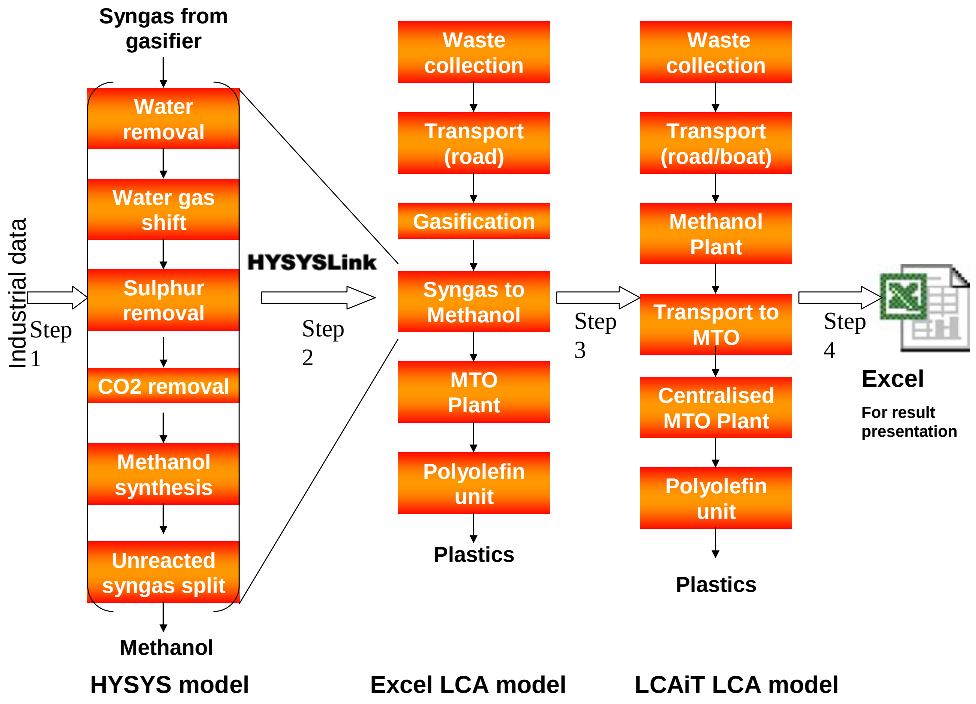


Figure 21: LCA-process modeling integration for the waste-to-plastics case study

The results from the HYSYS model were then exported (Step 2, Figure 21) to an Excel LCA model that includes input, output and emissions for each process step, normalised to the functional unit (1 kg of plastics). The process units gasification, MTO, transport and plastic production, were not modelled in HYSYS, and the process data were taken directly into the Excel model. The Excel model was used to calculate the emissions from the system. Although an extensive set of emission parameters were calculated and have been reported elsewhere (Nouri & Kaggerud 2005), only renewable and non-renewable CO_2 are reported here. The mass flows were then exported to LCAiT, an LCA software package (Step 3, Figure 21), to calculate the environmental impacts of the system using LCAiT databases. Finally, the impact assessment graphs together with the Life Cycle Inventories were exported to Excel files for LCA results presentation (Step 4, Figure 21).

From a process modeling perspective, biomass to plastics (BTP) and plastics waste to plastics (PTP) routes have been successfully simulated with different production system configurations (ex: hydrogen ratio improvement in syngas). Regarding environmental impact, many what-if scenarios have been assessed. Only LCA combined with process modeling allow for the CO_2 emissions to be tracked down where they are created: the quality of the syngas before the methanol synthesis is the key. Indeed, the gasification unit, with the air separation unit to produce oxygen, is the main emitter. A case with an improved gasifier for plastic waste shows significant improvements (cf. Table 9). The base case scenarios (shortly described in 3.1 and in Figure 15) show less CO_2 emissions for the biomass case, with respect to the non-renewable CO_2-equivivalents. The main reason for the lower CO_2 emissions in the biomass process is the lower oxygen use in that case.

Table 9: Summary of kg CO_2-eqv and waste per functional unit for the various scenarios.

Scenario		Renewable CO_2-eqv	Non-renewable CO_2-eqv	Waste per functional unit	
				Dry	As received
Base case	Wood Plastic	5.8 5.8	1.4 2.2	4.7 3.6	9.4 3.6
Improved gasifier*	Plastic	4.4	1.4	2.8	2.8 (1.4)**
H_2 added to syngas	Wood Plastic	3.5 3.5	1.1 1.7	3.4 2.7	6.7 2.7

*Oil slurry gasifier.

**50 % oil slurry in the treated material; 1.4 kg of waste plastics and 1.4 kg of oil per functional unit.

Moreover, the common base of process modeling could help organising the links between environmental assessments and cost assessments for the same process/product (see Footnote 4 in 1.2)

4.3 Process based cost model (PBCM)

As displayed as step 6 in Figure 1, the same process modelling thinking was applied to cost. A method for process based cost modelling (PBCM) developed at MIT was used for this (Kirchain and Field, 2000). The objective of PBCM is to map from process description to operation cost and to inform decision concerning technology before operations are in place (early design phase). The PBCM study was conducted in collaboration with researchers at MIT (Chiang, 2005) and the results are roughly in the range with the first cost assessments we have done (about $1000/ton is the cost of production a.k.a COP, for olefins). Moreover, for those who would not

agree with the assumptions done in the PBCM, it is very easy to just change them in the Excel sheets available as below. The process model will not change (it still will be oxygen blown gasification with methanol synthesis and MTO units), but the financial inputs (spot prices, utilities price, etc.) will:
http://www.esa.chalmers.se/Staff/bottomn_files/selim_files/MTO%20cost%20model.xls
http://www.esa.chalmers.se/Staff/bottomn_files/selim_files/WTM%20cost%20model.xls

4.4 Process based quantification of labor

As mentioned in section 2.6, we will now present a way to calculate the number of workers needed in a bioplastic plant, based on the BTP process. Indeed, measuring of factors of production consumed by the new technology is crucial. We will focus here on labor since it is one of the major issues linked to the use of biomass for energy or bioproducts purposes (see figure 22). The decision at a local level to invest in a bio project like BTP could be very influenced by the number of jobs created locally. We will present here a short example of such quantification using the BTP as a test object to estimate the jobs needed for producing bioplastics:

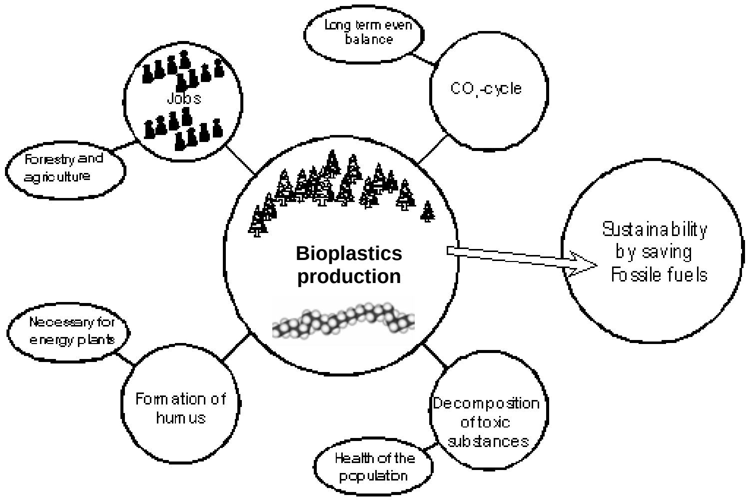
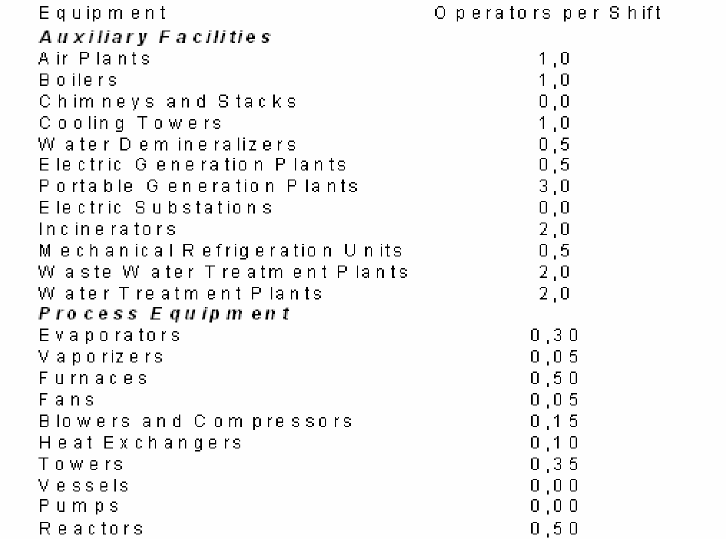


Figure 22: Categorised impacts of bioplastic production

The BTP plant concept is divided into the BTL plant (biomethanol production), the MTO unit with olefins production and the polyolefin unit. In a 548 ton/day biomethanol plant described by Ekbom et al (2003): the operation cost comprises staffing, insurance, land lease, and real estate tax. The personnel cost is calculated as 5 persons, 5 shifts and a regular staff of 15 persons. The assumed salary is €76,000/year including social costs plus a 50% and 20% overhead, respectively. Maintenance calculated as 3% of the cost of Equipment and Assembly and includes further spare parts, chemicals, and catalysts.

For the MTO plant, we will present a methodology based on process flowsheet analysis: using the following table and the UOP simplified process flowsheet we calculate the number of workers needed:

Table 10: Operators needed per shift for each process equipment (Turton et al, 1998)



Equipment	Operators per Shift
Auxiliary Facilities	
Air Plants	1,0
Boilers	1,0
Chimneys and Stacks	0,0
Cooling Towers	1,0
Water Demineralizers	0,5
Electric Generation Plants	0,5
Portable Generation Plants	3,0
Electric Substations	0,0
Incinerators	2,0
Mechanical Refrigeration Units	0,5
Waste Water Treatment Plants	2,0
Water Treatment Plants	2,0
Process Equipment	
Evaporators	0,30
Vaporizers	0,05
Furnaces	0,50
Fans	0,05
Blowers and Compressors	0,15
Heat Exchangers	0,10
Towers	0,35
Vessels	0,00
Pumps	0,00
Reactors	0,50

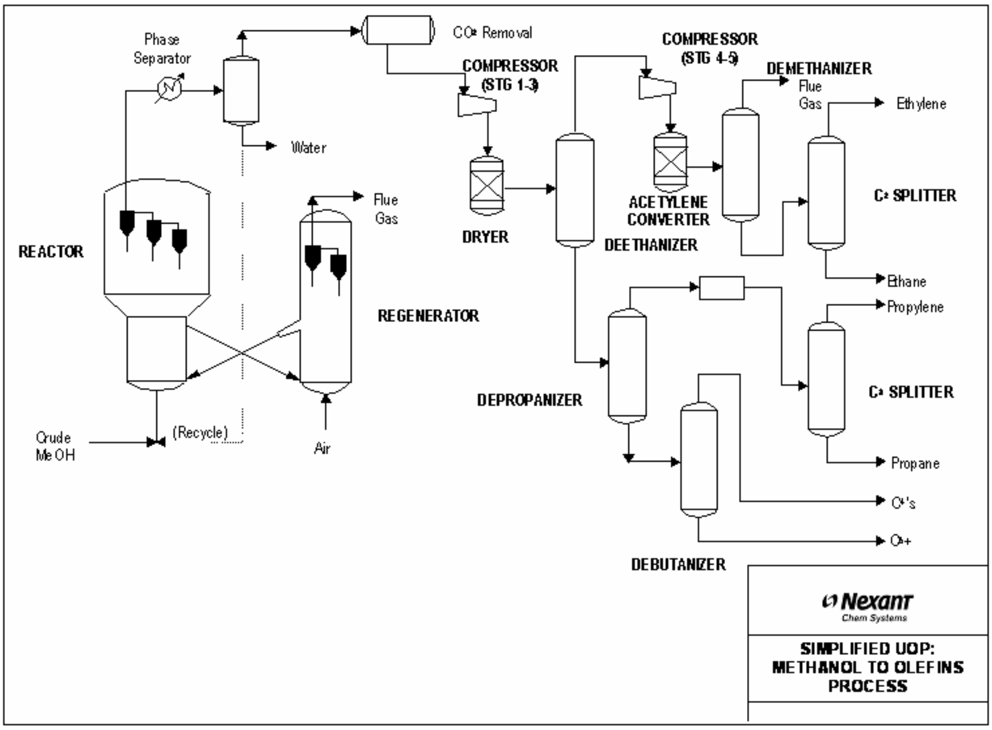


Figure 23: UOP MTO process flowsheet (Nexant 2003)

From table 9 and Figure 23, we have:
Reactor = 0.5 operator
Regenerator ~ furnace = 0.5 operator
Phase separator ~ heat exchanger + tower = 0.45 operator
CO2 removal (MEA) ~ tower = 0.35 operator
Compressor = 0.15 x 2 = 0.3 operator
Dryer ~ reactor = 0.5 operator
Depropanizer, debutanizer, demethanizer, deethanizer, C-splitters ~ tower x 6 = 0.35 x 6 = 2.1 operator
Acetylene converter (optional cf. Kvisle) ~ reactor = 0.5 operator
Total = 5.2 operators per shift

We chose 5 shifts (see Ekbom et al, 2003) and the same ratio of foremen and super than in the Nexant HDPE document (see table 11).
This lead to a number of 26 operators, 5 foremen and a super, so a total of 32 workers.

The polyoefin unit workforce is given by Nexant chem. System for a HDPE unit from Borealis:

Table 11: HDPE Borstar technology key data (Nexant 2003)

HDPE
Basis: USGC, Fourth Quarter, 2001

Table	A34
Licensor	Borealis
Process Name	BORSTAR
Technology	Slurry/Gas-phase
Product	HDPE Bimodal Film
Comonomer	Butene-1
Capacity, KMT/YR	250
, MM LB/YR	551
Capital Investment, $MM	
ISBL	80.5
OSBL-Storage & Packaging	22.4
OSBL-Other	36.6
TOTAL FIXED INVESTMENT, $MM	**139.5**
Other Project Costs	34.9
Working Capital	**18.4**
TOTAL CAPITAL INVESTMENT	192.9

Cost of Production	**$/unit**	**units/lb PE**	**$/lb PE**	**$/MT PE**
Raw Materials				
Ethylene, lb	0.229	0.9920	0.227	501
Butene-1, lb	0.253	0.0200	0.005	11
Hexene-1, lb	0.347			
Hydrogen, lb	2.576	0.0002	0.001	1
Solvent, Gal	0.957			
Propane, Gal	0.343	0.0024	0.001	2
Isobutane, Gal	0.396			
Hexane, lb	0.137			
Catalyst & Chemicals			0.0074	16
Extruder Additives			0.0087	19
Total Raw Materials			**0.250**	**551**
By-product credits				
PE, low mw, lb	0.100			
Total by-product credits				
Net Raw Materials			**0.250**	**551**
Utilities				
Power, kWh	0.046	0.2250	0.010	23
Cooling water, MGal	0.088	0.0150	0.001	3
Steam,600 psig, Mlb	5.388			
Steam,200 psig, Mlb	4.799	0.0002	0.001	2
Steam,50 psig, Mlb	4.726			
Inert gas, MSCF	1.458	0.0014	0.002	5
Fuel gas, MMBtu	2.530			
Total Utilities			**0.015**	**32**
Variable Cost of Production			0.264	583
Direct Cash Cost	$/man	# men		
Labor	40 100	28	0.002	4
Foremen	45 500	5	0.000	1
Super.	54 900	1	0.000	0
Maint. @ % ISBL + OSBL S&P		2.7	0.005	11
Direct ovhd. @ % labor+super		45	0.001	3
Total Direct Cash Cost			0.009	19
Allocated Cash Cost				
Gen'l. plant ovhd. @ % direct cash cost		60	0.005	12
Ins., prop. tax @ % total fixed inv		1.0	0.003	6
Environmental costs @ % total fixed inv		0.5	0.001	3
Total Allocated Cost			0.009	20
Total Fixed Costs			0.018	39
TOTAL CASH COST			**0.282**	**622**

This give a number of 34 workers for this HDPE borstar unit for a 250 000 metric ton per year, thus – using again the Nexant data – it give a number of 8 workers (6 workers, 1 foremen and 1 super) for a BTP plant based on methanol production.

The number of workers for the Biomass to polymer (182 t/day polyolefin output) plant would be then around 80 (see table 12).

Table 12: Number of worker needed for a bioplastic manufacturing plant.

Process islands	Number of workers
Methanol from biomass plant	40
Methanol to olefin unit	32
Polyolefin unit	8
Biomass to polymer plant	80

5 Main results and discussion

During this project, due to a rich environment for research (research diversity at ESA, collaboration with MIT, CPM at Chalmers, PLUS at Chalmers, IDA at Chalmers, etc.) a lot of results both numerical and methodological have been carefully collected. The main results in terms of potential routes, assessment results in terms of comparisons and methodology issues will be discussed, and the details may be found in paper I and II apart from reports (see Nouri & Tillman, 2005) and website (www.esa.chalmers.se/Staff/bottomn_files/Selim.htm).

5.1 Methodological feedback: technology screening and life cycle assessment

For emerging technologies, environmental assessment like life cycle assessments are often following technical screening and thus are often influenced by them. The risk that information from technology screening will uncritically be used directly in the following life cycle assessment is thus great. To reduce this risk a methodology has been developed and implemented on the case of bioplastics (see paper II). It will be shortly presented here.

5.1.1 Technology screening weaknesses for environmental assessment use

Most technology screening reports are not intended to be used directly for environmental assessments. They present a multitude of information that need, therefore, to be “organised” if they are to be used for such assessments. Moreover, due to their inherent context, they may “miss” some information that is relevant in environmental assessments. Let us explain what we mean by “not organised” or “missing” information and the consequences for environmental assessments.

“Not organised” refers to a case where information is mixed and not evaluated. Often, information about all types of technologies is blended (no clearly defined timeframe: technologies used today, near-future ones and very futuristic technologies, organisational backgrounds: academic, industrial, military…). It is therefore easy to mix technologies that are incompatible from an environmental assessment perspective.

“Missing” information is another classic mistake when it comes to use of technology screening for environmental assessments. The most common case being the omission of relevant alternatives like in the last IPTS report about bioplastics (Wolf et al, 2005), where thermochemical processes are omitted.

5.1.2 Methodology

The purpose of this methodology is to be able to use technology screening for environmental assessments like LCAs. It is a 6 steps bottom-up oriented - from basic structures such as polymer precursors, to industrial networks – methodology (see table 13):

Table 13: Six steps methodology to organise information in technology screening

Steps	What is done	Why is it done
Step 1	Define feedstock, products and time horizon	This step is fundamental in order to set the boundaries of what we are dealing with. It explains on what grounds further any chemical intermediates may be selected.
Step 2	Map routes from feed stock to products	It helps decreasing the risk to “miss” potential process routes in the beginning.
Step 3	Gauge maturity of the technology	This organises information about the existing routes and distinguishes between routes which have different maturities of the technology, such as those already commercial, those in a near future and those that need much more development
Step 4	Assess technical activity levels	This step helps organising information regarding development intensity of processes in terms of volume of technological activities (e.g. patenting). It gives arguments for potential processes.
Step 5	Gauge and map routes according to potential for integration with other sectors	This step organizes information regarding the potential of some routes with respect to their integration with other sectors and the mapping

		helps identifying intermediates that have a high level of integration potential with those other sectors. It gives arguments for cross-sector processes.
Step 6	Gauge public expectations	This step organises information in terms of expectations on certain routes. It gives arguments for fashionable processes.

Basically, mapping helps avoiding omissions and gauging helps organising information.

For illustrative purposes, we choose to apply our methodology to bioplastics (plastics produced from biomass). This is an appropriate case study due to its inherent complexity in terms of technology but also in terms of environmental expectations. This inevitably leads to many technology screenings and a huge demand for environmental assessments, like LCA; the risk that technology screening is uncritically used for environmental assessments is, therefore, great.

5.1.3 Biomass to plastics example

The application of the methodology to bioplastics was very conclusive. Indeed the difference between an LCA with or without our methodology is striking. For instance without, using technology screening information as such, for the environmental assessment of the production unit of one of the biopolyolefin intermediate, the LCA results are 12 g of CO2eq/kg polymer emitted whereas we found 775 g of CO2eq/kg polymer emitted for this unit using our methodology (see figure 24). This kind of differences has a lot of importance for instance if dominance analysis of the BTP process is performed.

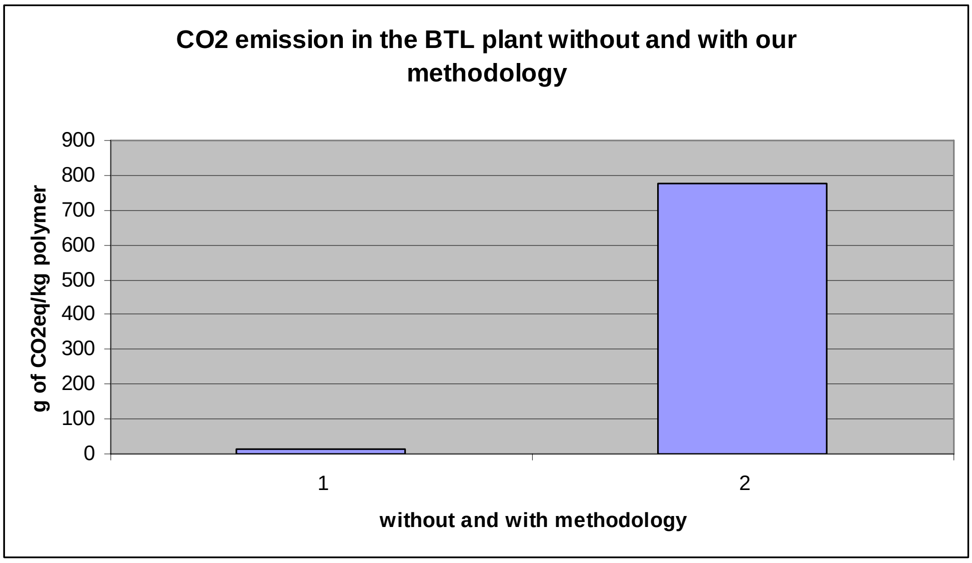


Figure 24: Green House Gases emissions in the BTL unit for the BTP process (cradle-to-gate) with (2) and without (1) the methodology

The difference in this case, is due to the fact that without the methodology, the risk of using very futuristic scenarios information, like in case (1), is higher.

5.2 Potential routes

From the biopolymer background, we have identified two types of routes as potential ways to produce bioplastics: thermochemical or biotechnology based processes. Within the pool of potential and existing routes to bioplastics, some intermediates and bioplastic precursors have shown special attractiveness (integrated to industrial network, popular, etc.). The data collected about those intermediates towards bioplastics enable to make a mapping of all potential routes (see paper II).

The biomass to plastic mapping allows a direct and global perspective of the bioplastics production issues. Indeed, by identifying the main intermediates to bioplastics, it allows to identify the possible links with other industrial sectors - like Biofuels - or products. For instance, the Biomass to Liquid (BTL) and Methanol to olefins (MTO) processes showed in the bioplastic process mapping (see figure 14) have been identified and studied in many details. A mapping of these specific processes compared to others (like GTL) has even been performed (see http://www.esa.chalmers.se/Staff/bottomn_files/Selim.htm#Maps1).

The most interesting routes from our analysis in paper I (cf. figure 14) are the following:

1. Wood waste to syngas to ethanol to ethylene to polyethylene
2. Wood waste to syngas to methanol to DME to C2/C3 to Polyolefins
3. Wood waste to syngas to DME to C2/C3 to Polyolefins

In all these routes, there is no need to separate the cellulose from the lignin. This is a big advantage compared to cellulosic ethanol production route, where only the cellulose can be transformed into ethanol via the sugar route. Indeed, countries with rich lignocellulosic feedstock could monetize it better by using the syngas route (see appendix 5).

It is interesting to see that these syngas based routes are the routes we choose to study in our project from the beginning (see Nouri & Tillman, 2005). Moreover those routes were worth studying in details since they seem to have been forgotten in some bioplastics related studies (Wolf et al, 2005).

Moreover, despite our focus towards cradle-to-gate research – we have indeed modeled production processes mainly – we have kept in mind that the waste management part could greatly influence the production one. Indeed, during our modeling of Plastic-to-plastic process (see Nouri & Kaggerud, 2006) we saw that the connection between production and waste management is essential. In addition, as mentioned by PlasticsEurope, the misfit between a production system like compostable bioplastics and a waste management one, like incineration could lead to global increase of green house gases. Therefore, the identification of potential routes towards bioplastic is a key to technology evolution scenarios. For instance, the scenario described by PlasticsEurope in 2.1.1 would never happen in the first place with bioplastics from a BTP process, since the bioplastics produced have the same energy content than their fossil based counterparts.

5.3 Assessment Results

Within the Biofuel business, both biotechnology based processes (e.g. cellulosic ethanol) and thermochemical processes and especially syngas based processes are quite popular, with many projects and actors involved. However within the biopolymer business, thermochemical processes are almost invisible (see Wolf et al. 2005). We showed in our research that not only the thermochemical processes and syngas based ones are potentially feasible (technology is available and pilot plant are dispersed around the world) but on top of that, that they would perform as well or better in terms of environmental impact and cost than their biotechnology based counterpart such as PLA (see table 14).

Table 14: BTP production outperforms both biotechnology based bioplastics and existing polymers

	COP $/MT	**kgCO2 eq/kg**	**MJfossil/kg**
Polylactic acid	**1100**	**1.83**	**57**
Biopolyolefin	**770**	**0.3-1.4**	**56.5**
Polyethylene	**880**	**5**	**80**

5.4 Methodology feedback: combining LCA with process modeling

We will now present the way we have combined LCA with process modeling for the BTP example. More generally, we linked LCA and process modeling using HYSYS and LCAiT as software. After creating a process model, the results from the HYSYS model were exported using HYSYSLink, a dedicated HYSYS add-in, (2 in Figure 25) to Excel which served as platform between process modeling and LCA software. The imported results from the HYSYS model were normalised to the functional unit, calculating the mass and energy flows per functional unit to make them easier to process with the LCA software. The mass flows were then exported to LCAiT (3 in Figure 25) to calculate the environmental impacts of the process. Finally the impact assessments graphs together with the Life Cycle Inventories were exported to Excel files for LCA results presentation (cf. 4 Figure 25). Choosing the same platform - here Excel - could easily allow to close the information loop (cf. 5 Figure 25) making the system dynamic. One can then conceive an integrated process evaluation system that unifies process simulation, design and environmental performance analysis/monitoring into one application. This was however not implemented in this project.

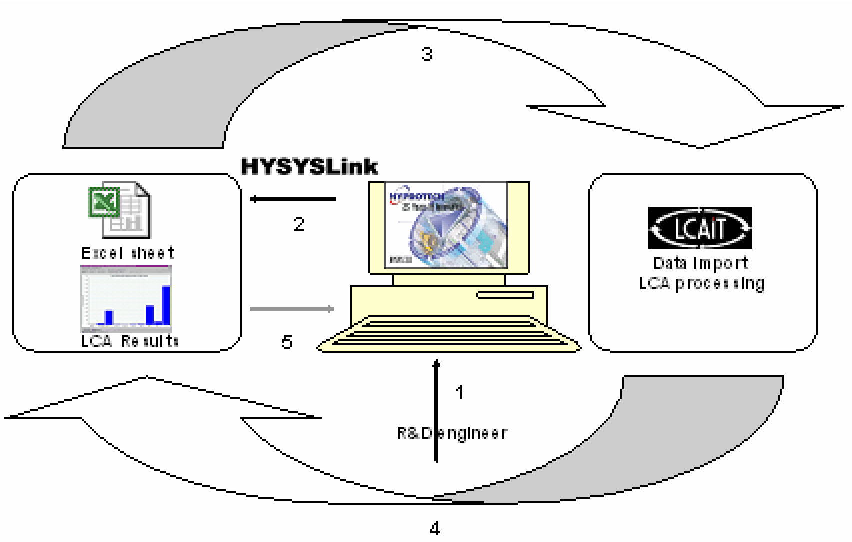


Figure 25: Data flows for LCA-process modeling combination

6 Conclusions

The main conclusions of this thesis are threefold: general, about sustainability and about methodology.

General conclusions from the (bio)polymer background:

- From a consumer perspective, most of the bioplastics proposed today by bioplastics producers are not solving the main problem.[12] Five billions plastic bags are still littered every year and some of the bioplastics proposed today (like PLA) are not biodegradable in a sense that they will leave no trace if littered. They are therefore missing the target. The bioplastic industry is misleading the consumer by advocating new advantages that are either producer oriented (security of feedstock, marketing) or of secondary importance (climate change mitigation, compostability)[13]. Other alternatives however exists that could solve the

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[12] We assume that the main environmental issue posed by conventional plastics is their long time to degrade. (see http://www.assemblee-nationale.fr/12/propositions/pion1807.asp and http://en.wikipedia.org/wiki/Plastics#The_environment)

[13] We, of course, do not say that climate change is of secondary importance; but for the particular case of plastic industries, that it is not the main environmental threat posed by those industries. Only 4% of total energy source in the US are for plastics.

main problem of plastic littering. Those are real degradable plastics (either from fossil fuel or not) that could fit the existing waste management systems (see Nor-X additives or equivalents).
- from a plastic manufacturer perspective, the shift to alternative feedstock seems more important than ever. White biotechnologies seems the way to go for plastic production (the growth potential of those industries is enormous), but technology transfer from GTP projects (see MTO technologies) to the biomass based industry is potentially feasible when looking at thermochemical processes. Moreover, the rebirth of ethanol as a global fuel commodity could also relaunch interest in ethanol dehydration to produce ethylene and then polyolefins.

Sustainability conclusions: bioplastics outperform in general conventional plastics regarding the energy use and the green house gases emissions during their production. One can say that if sustainability is here reduced (for simplicity reasons) to environmental and cost issues, then bioplastics seems more sustainable than their fossil fuel counterparts with an especially good performance for plastics produced via the BTP route.

Methodology conclusions: Life cycle thinking has again demonstrated its efficiency in grasping all the potential issues included in bioplastics production, from electricity systems to logistic issues. Our research has help to identify the risks linked to combining technology screening information and LCA and to find a methodology to combine them properly (see paper II). Moreover, the combination of LCA and process modeling has been very fruitful (see paper I) with a tracking down of the emissions trough the process and where they are created. The combination of process modeling and LCA software may and should disappear in a near future with the integration of environmental impact assessment within the process modeling software suite, like it has been done with economic tools. This would be logical when following the life cycle thinking strategy spreading within big companies, from R&D to marketing.

7 Further work

On a short term perspective, what could be done is a consolidation of results, both environmental with the process modeling LCA combination (one can think of adding better models of the gasification and MTO unit with .hsc files) and cost oriented with an updated PBCM for the BTP route. The same kind of assessment could also be done for the other biomass to plastic route identified.

In a longer term perspective, the trend to have add-ons to process modeling software like economics add-ons or environmental add-ons could be concretised with, for instance HYSYS as a playground for chemical process modeling. Existing economics add-ons could be combined to new designed LCA add-ons to increase the efficiency of such an assessment tools for emerging technologies and processes.

Finallly, the close links between production systems and waste management ones – pinpointed using life cycle thinking – should also be studied carefully in future research to avoid misleading strategies and unwanted environmental impacts.

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8 Appendix 1: Natural gas flaring worldwide

Despite the world huge demand increase in fossil fuels, the resource management of those fossil fuels and particularly natural gas, is very poor. Indeed we are still flaring more and more natural gas every year (see figure 26). Organisations like the World Bank have launched programs to monitor and reduce this phenomenon and their experience and models could probably be also used for a future global biomass based industry (Mouton, 2005).

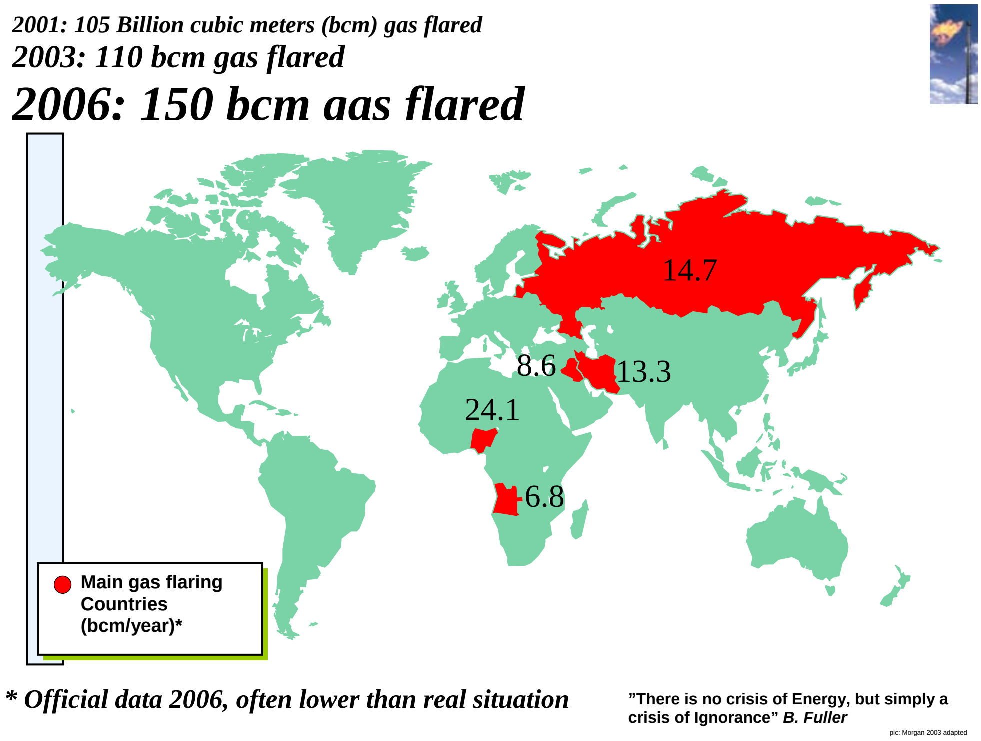


Figure 26: Increasing of gas flaring world wide from 2001

9 Appendix 2: ethylene hydration and ethanol dehydration

In some case, it could be worthy to produce ethanol from ethylene dehydration (see COP figure 27). This is mainly done in Saudi Arabia, where ethylene from ethane cracking is cheap and abundant.

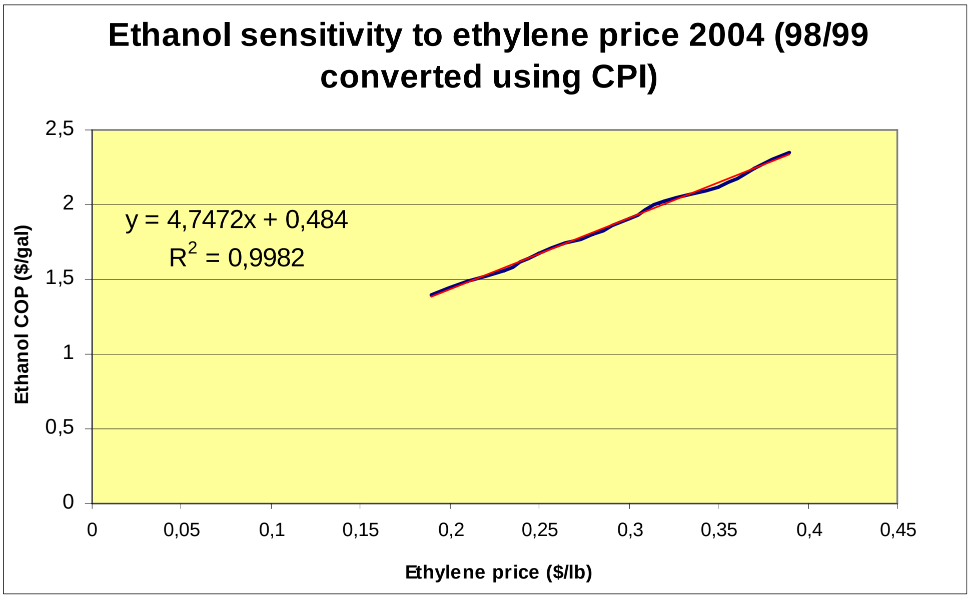


Figure 27: Cost of producing ethanol from ethylene depending on the ethylene feedstock (98/99 data converted using consumer price index or CPI)

In some other regions, it could be worthy to do just the opposite and to produce ethylene from ethanol dehydration (see COP figure 28). This is done mainly in Brazil, where ethanol from sugar cane is cheap and abundant.

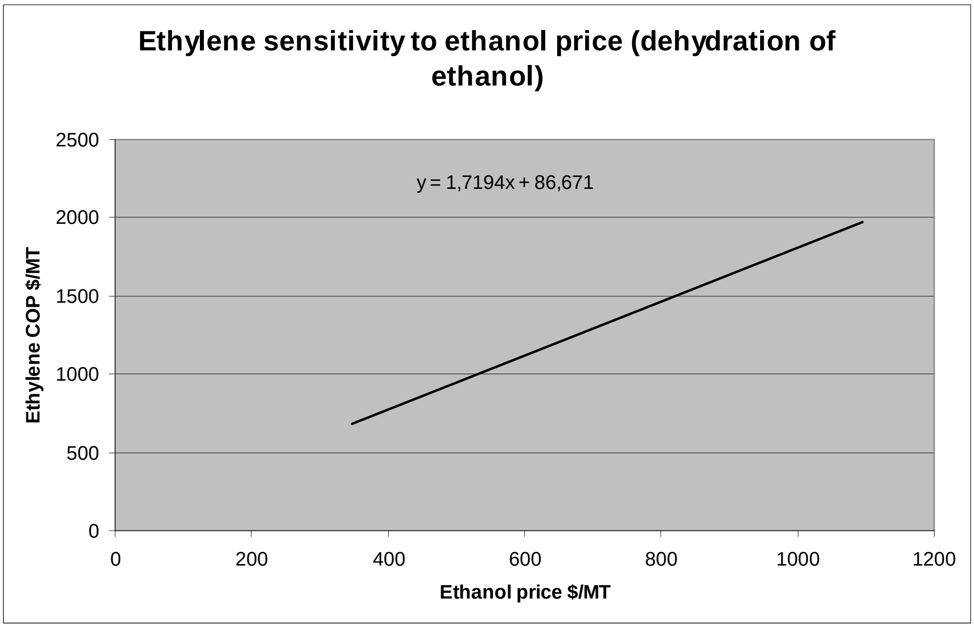


Figure 28: cost of producing ethylene from ethanol dehydration depending on the ethanol feedstock price

10 Appendix 3: parallel between natural gas and biomass business

Table 15: The parallel between natural gas and biomass is striking:

Natural gas	Biomass
Stop natural gas flaring	Stop waste littering
Methane tanker, LNG, gas infrastructures	Waste transport, biomass refining, treatment infrastructures
Electricity-Gas sector cooperation	Electricity-waste market actors cooperation

11 Appendix 4: stream lined LCA calculations

GHGs emissions for the BTP routes have been calculated as follow:

Wood waste collection and chipping:
The wood waste considered is forest residual from commercial forestry (Edwards 2003).

This gives net GHGs emissions (emissions from biomass sources not accounted) of 0.7 g CO2eq/MJf (MJf stands for MJ fuel, here MJ methanol, EDWARDS 2003). Since methanol has a calorific value of 20 MJ/kg, the net GHG emitted are 0.7 x 20 = 14 g CO2eq/kgMeOH. Moreover, 3 kg of methanol are needed to make 1 kg of polymer, so 14 x 3 = **42 g CO2eq/kgPolymer** is emitted during collection and chipping of wood waste.

Transport to gasification plant:
The average transport distance for forest residual collection is about 50 km (EDWARDS 2003). Assuming that road transport is chosen - worst case scenario since a combination of shipping and road transport is more likely to happen for a plant that size - emissions are 0.7 g CO2eq/MJf (EDWARDS 2003) so **42 g CO2eq/kgPolymer** is emitted during transportation to the plant.

Methanol plant:
Emissions from the bio-methanol plant (gasification and methanol synthesis) have been assessed and are about 0.2 g CO2eq/MJf (EDWARDS 2003). As a comparison, it could be mentioned that 11.7 CO2eq/MJf are emitted for methanol, from natural gas (EDWARDS 2003).
It represents 4 g CO2eq/kgMeOH and thus about **12 g CO2eq** emitted per kg of polymer produced.

MTO plant:
Industrial data from UOP/Hydro give and estimation of GHG of about 200 gCO2eq/kg olefin produced. This data is corroborated by the extrapolated data for the Ifp's MTO process (Joosten 1998) with GHG emission of about 280 gCO2eq/kg olefin produced. Those CO2 emissions were calculated from the combustion of the process output fuels. CO2 emissions caused by the combustion of the extra fuel needed are excluded. Since all the carbon comes from biomass in the process, the only net emissions of GHG accounted are those from the combustion of extrafuel (assumed to be oil). The MTO required about 1.33 MJ extrafuel per kg of olefin produced (Joosten 1998), thus about the same per kg of polymer produced. The combustion of 1MJ of oil emits about 75.8 g of CO2

(Baumann, Tillman 2004) and the extraction/processing and transport 6 g of CO2, thus the MTO net CO2 emissions are about **107 g of CO2** emitted per kg of polymer produced.

Polyolefin unit:
The polyolefin unit global warming potential emissions can be found in the literature (Baumann Tillman 2004) and the total emissions are about 49.7 g CO2eq/kg of polymer produced for the air emissions and 8.6 g CO2/kg of polymer from the combustion of fossil fuel (assumed to be oil) needed and 6 g of CO2 for its production. The total global warming potential emissions are **64.3 g CO2eq/kg** of polymer produced. Here again we use a worst case scenario by taking the data for an HDPE polymerisation unit which consumes more energy than a PP one and by assuming that all the carbon from the flaring is from fossil origin, which may not be true.

Energy use for the BTP route has been calculated as followed:

Wood waste collection and chipping:

The total primary energy consumed for waste collection and chipping is 0.06 MJ/MJf of methanol produced (EDWARDS 2003). Since methanol has a calorific value of 20 MJ/kg, the energy used is 0.06 x 20 = 1.2 MJ/kgMeOH. Moreover, 3 kg of methanol are needed to make 1 kg of polymer, so 1.2 x 3 = **3.6 MJ/kgPolymer** is used during collection and chipping of wood waste.

Transport to gasification plant:
Assuming that road transport is chosen, the total primary energy consumed is 0.01 MJ/MJ methanol (EDWARDS 2003) so **0.6 MJ/kgPolymer** is consumed during transportation to the plant.

Methanol plant:
Total primary energy consumed for the bio-methanol plant (gasification and methanol synthesis) has been assessed and is 0.96 MJ/MJ methanol (EDWARDS 2003).
It represents 19.2 MJ/kgMeOH, and thus about **57.6 MJ** total primary energy is consumed per kg of polymer produced. The process energy consumed is assumed to be electricity and is about 0.1 MJ/MJ methanol (cf. fig 26) or about 6 MJ electricity per kg of polymer produced.

MTO plant:

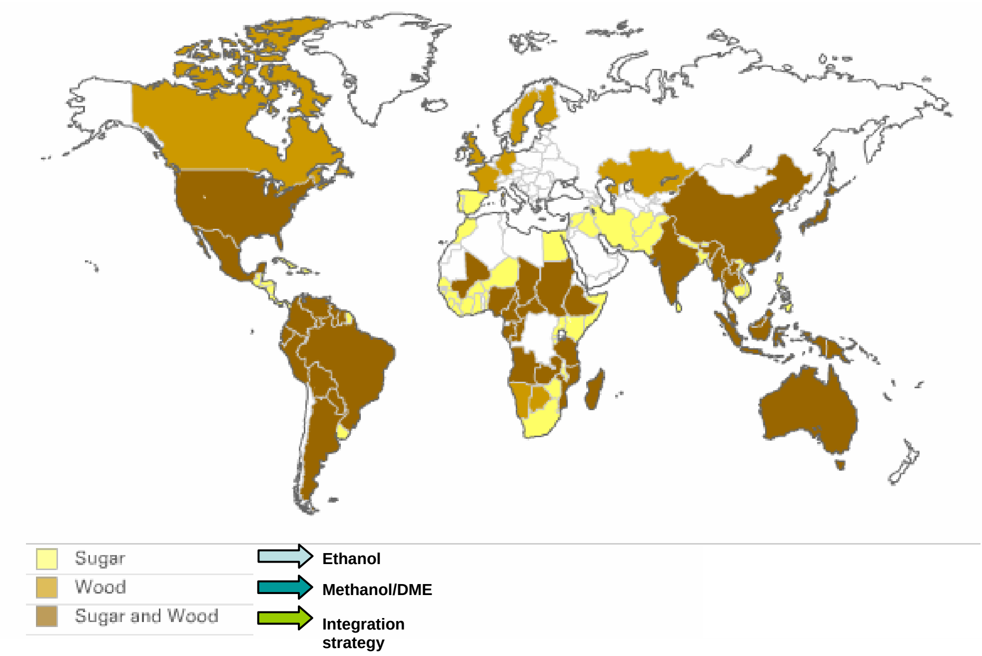
The MTO process uses roughly 0.3 MJ of electricity, 2.8 MJ of fuel and 1.1 MJ of high pressure steam to run and produce 2.11 kg of olefins (Joosten 1998) thus about 0.14 MJ of electricity, 1.33 MJ of fuel and 0.52 MJ hp-steam are used per kg of polymer produced. If electricity is generated with a 35% efficiency (E.U-Mix EDWARDS 2003), the primary energy associated to 1 MJ of electricity is 2.86 MJ. The total primary energy associated to the process is then 2.25 MJ per kg of polymer produced.

Polyolefin unit:

The polyolefin unit energy consumption can be found in the literature (Baumann, Tillman 2004) and the total energy used is about 6.6 MJ electricity per kg and 2.2 MJ of fossil fuels per kg of polymer produced for LDPE, and 2.1 MJ electricity per kg and 0.11 MJ of fossil fuels per kg of polymer produced for HDPE. If electricity is generated with a 35% efficiency the primary energy associated to 1 MJ of electricity is 2.86 MJ. The total primary energy associated to the polymerisation process is then 2.1 x 2.86 + 0.11 = 6.12 MJ per kg of HDPE produced.

12 Appendix 5: Wood alcohol and alcohol

Ethanol is also called grain alcohol whereas methanol is called wood alcohol. The reason is that depending on the feedstock it is easier to produce one or the other. Indeed, to produce ethanol from sugar is very easy and grain can also be easily transformed into sugar. Therefore, depending on the sugar/grain availability geographically, it could be easier to produce ethanol or methanol/DME (see figure 29):



Source: Dynamotive 2006

Figure 29: The geographical availability of sugar or wood leads to strategies of producing grain alcohol or wood alcohol, or to integration strategies.

Environmental implications of syngas-based bioplastics and dedicated waste management process

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Abstract

This paper examines processes for converting biomass to plastics (BTP) and plastics to plastics (PTP) from an environmental perspective. The technologies evaluated are thermochemical conversion of the raw material into plastics and already exist at a pilot or demonstration unit scale. The core strategy is to take the biomass or plastic waste through gasification, methanol production, methanol to olefins (MTO) and finally plastic production. The environmental attractiveness of these emerging technologies is evaluated using a combination of process modelling and life cycle assessment (LCA) methodology. Several tools and simulation software programs have been combined to carry out the study, including HYSYS, LCAiT and Excel. Various improvements of the processes have been evaluated with respect to greenhouse gas emissions. The most important outcomes of the study include:

- Production of plastic waste from biomass and plastic waste seems to be technically feasible using the BTP and PTP processes, respectively.

- The gasification unit, with the air separation unit to produce oxygen, is the main contributor to CO_2 emissions. A case with an improved gasifier for plastic waste shows significant improvements.

- Another option to improve the BTP and PTP routes is the addition of hydrogen. This is environmentally friendly if hydrogen is available as excess hydrogen or as a by-product from other processes. Such hydrogen exists in quite large quantities and may be used not only for fuel purposes but also for improving bioproduct production efficiency.

- The method, which combines LCA and process modelling, enables an effective early-design phase evaluation.

Keywords: Methanol-to-Olefins (MTO); syngas; Life Cycle Assessment; process modelling; biopolymers

1 INTRODUCTION

In these times of high energy demand, waste monetization strategies for both fuels and materials (i.e. plastics), are highly appreciated. Wood wastes from forest and pulp-and-paper industries, as well as plastic wastes, represent interesting feedstocks for syngas-based processes that can lead to numerous products, including plastics production. Those processes could help to monetize waste, thereby reducing the amount of waste, whilst at the same time saving fossil fuels and mitigating climate change. However, the concept of waste-to-plastics and, more particularly, the plastics-to-plastics (PTP) route needs to be assessed in terms of environmental impact and chemical engineering. Indeed, previous studies [1], [2] have identified syngas-based processes capable of producing polymers using existing technology (pilot plant scale or demo plant scale minimum). Those technologies can be built within 5 years.

The purpose of this study is to model the production of plastics from wood waste or plastic wastes, to evaluate the environmental impact of the different process configurations and to distinguish the pros and cons of each. The rationale for carrying out the study is twofold; to evaluate different design alternatives at an *early design phase* for production of plastics from waste, and to determine whether or not it makes sense, from an environmental point of view, to produce plastics from waste plastics or wood waste.

2 METHOD

The method followed was the construction of potential process configurations using a combination of technical knowledge of BTP and PTP processes and available literature. The environmental impact was subsequently evaluated using a combination of streamlined life cycle assessment (LCA) and data from HYSYS models.

Different ways to produce polyolefins from waste using syngas technologies were modelled and evaluated with respect to environmental performance. The results were used to identify the best option for production of polyolefins from waste plastics or wood waste by modifying process options such as technology, plant configuration and location. In addition to identifying the best options for each of the waste sources, it was interesting to compare the differences and similarities of the two options. The different composition and nature of the two feedstocks require different configurations and, to a certain extent, different technologies. One example is the chlorine content in the plastic waste, which is not present in biomass at all. Special attention was also given to the distinction between the CO_2 originating from the waste and CO_2 from other sources, such as electricity production and fuel for transport.

The initially modelled processes includes 7 main steps (Figure 1): the waste handling, the gasifier, the gas cleaning section, the water gas shift, the methanol synthesis, the methanol-to-olefins unit and the polyolefin unit.

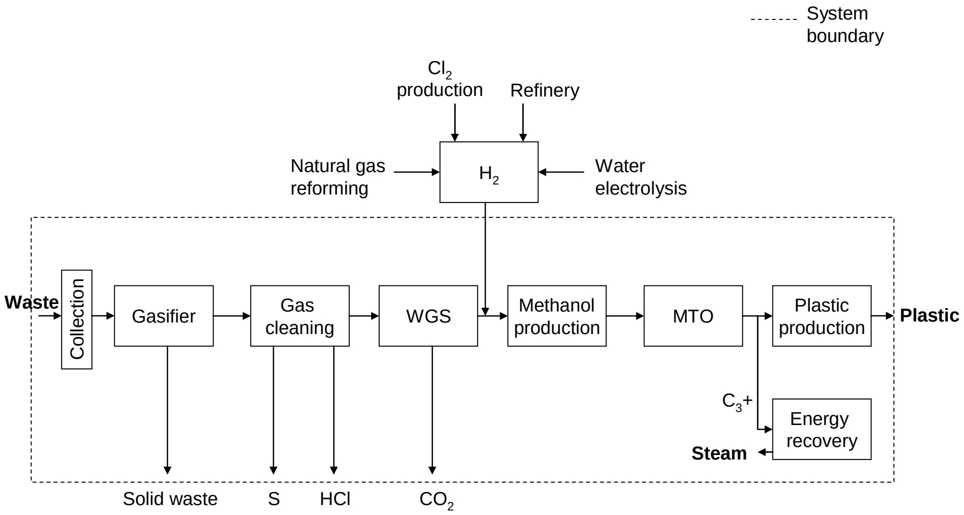

Figure 1: Block diagram for production of plastic from biomass (wood waste) and plastic waste, the system boundary is shown as the dotted line.

In the model, a cradle-to-gate perspective was used. Therefore, neither the use phase of plastics nor plastic waste production were included. Neither is the forestry that produces wood waste as a by-product. The technical system takes into account the consequences of the different process configurations to produce polyolefins, from the waste collection to the output of the polyolefin unit.

Many process and market parameters are closely linked to the location of production facilities (electricity production, product demand, waste availability, transport, etc.). The modelled process train, including electricity production, was assumed to be located in Western Europe, using an E.U electricity mix. It is an advantage for the process to be located close to a hydrogen source: near a chlorine plant, a refinery, a methanol or ammonia plant [3]. In addition to the Western European location, a localisation in Eastern Europe will also be studied in the sensitivity analysis.

Since this study is only concerned with processes that can be commercialised within 5 years, potential future developments such as electricity generation via fuel cells are not considered. An advantage of this is that data availability is both better and more consistent. Data is taken from technical reports and published papers.

2.1 LCA modelling choices

The functional unit (FU) is 1 kg of plastic, of which 0.68 kg is HDPE and 0.32 kg is PP, since the Methanol-To-Olefin (MTO) process studied produces this proportion of ethylene and propylene. For CO_2 accounting, since the configuration changes have direct impact on green house gases emissions, it is important to account the carbon that comes from the feedstock (wood or waste plastics) separately from greenhouse gases emanating from energy systems or logistics. For practical reasons, the term renewable carbon emissions has been used for all carbon originating from the feedstock, irrespective of whether it is plastic waste or wood waste. Of course, CO_2 emanating from recycled plastics today is fossil in origin, but the terminology chosen a) allows for separating feed-stock CO_2 from other and b) could be said to simulate a situation where the recycled plastics are made from renewable sources.

Assignment of the CO_2 emissions

To assure that the **CO_2 emissions are correctly assigned to the unit where the emissions are formed**, the following allocation has been used for renewable CO_2:

Gasifier = *All CO_2 out of gasification reactor*

Shift = *All CO_2 out of WGS reactor - Gasifier*

Steam = *All CO_2 from combustion of flue-gas from methanol reactor*

MTO = *All CO_2 from reactor (regeneration of catalyst) +*

Combustion of off-gases (C_{5+}, H_2 and CO)

The traditional LCA approach, with assignment to the unit where the emissions occur, does not provide information of where the emissions originate. With the approach shown above, the **CO_2 is assigned to the unit where it is formed** and consequently, the results can be used to identify requirements for improvement in process development phases.

The production of capital goods, means of transport and buildings were not considered in this study.

2.2 Combination of process modelling software and LCA

To evaluate the environmental performance of the plastic production process from alternative feedstocks (wood waste or waste plastics), several technical and environmental methodologies and simulation software programs have been combined. This includes process modelling and LCA software packages, the combination of which gave the results presented and discussed in this paper.

Process modelling software packages are tools used by managers and engineers to determine optimum designs and to link business objectives with process design. They allow for the simulation of different process designs, specification of process equipment, evaluation of the effects of changes (feed, equipment etc) on the process and the assessment of process deficiencies. They also offer modules where the financial outcome of the process may be projected. However, these software packages assess environmental issues only in a very limited way. Energy use and other resource consumption processes such as feedstock are modelled, but they do not allow for the modelling of emissions to the natural environment, and hence are unable to determine environmental impact. Therefore, the software packages do not support the modelling of what-if scenarios with respect to environmental aspects. This is rather surprising, given the strong development of LCA approaches during the last decade and the chemical engineering roots of LCA.

LCA and process modelling were linked in this project. HYSYS was used to simulate a waste to plastics process and the results were then exported and integrated in an LCA model in order to calculate the environmental impact of the process. Variations of the base cases such as changes of energy systems, logistics, plant configurations, etc. were then simulated in a series of sensitivity analyses.

Gasification models are complex. For both simplicity and practical reasons, the gasification step was not included in the HYSYS model. Instead, data was taken from the literature. For the subsequent steps, a HYSYS model was built based on industrial data (Step 1, Figure 2). The model takes the raw syngas from the gasifier as an input and treats it all the way to methanol. The steps in the HYSYS model were the following (Figure 2):

- Water removal from the syngas, done by component splitter.
- Water gas shift (WGS) as a two-stage process, with addition of water to obtain a H_2/CO-ratio of 2 after the WGS.
- Removal of sulphur done by a component splitter using the same split fraction for all scenarios.
- Removal of CO_2 by two component splitters, where the first one is “recycle gas” to the biomass gasifier, and the second is “flue gas.” For plastic waste, the outputs from the first and second splitter are classified as “flue gas” since no recycle gas is needed in the gasifier.
- Reaction of cleaned syngas to methanol (methanol synthesis), at a conversion rate of 92% [4]. The reactor is followed by a component split of methanol, water and non-reacted syngas. The unreacted syngas is used as fuel gas in the steam island.

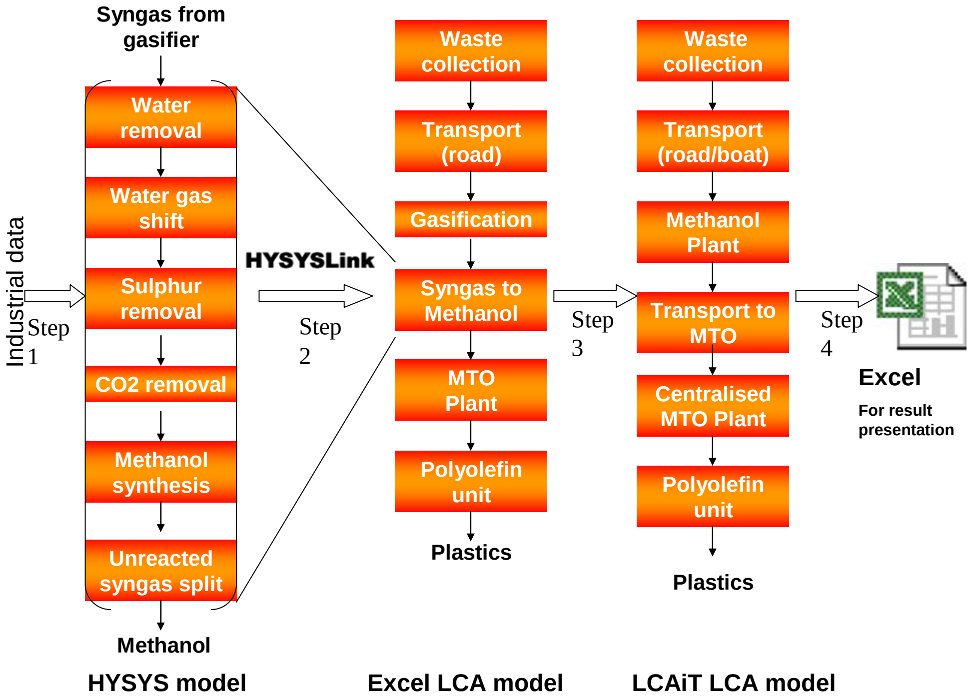

Figure 2: LCA-process modelling integration for the waste-to-plastics case study

The results from the HYSYS model were then exported (Step 2, Figure 2) to an Excel LCA model that includes input, output and emissions for each process step, normalised to the functional unit (1 kg of plastics). The process units gasification, MTO, transport and plastic production, were not modelled in HYSYS, and the process data were taken directly into the Excel model. The Excel model was used to calculate the emissions from the system. Although an extensive set of emission parameters were calculated and have been reported elsewhere [5], only renewable and non-renewable CO_2 are reported in this paper. The mass flows were then exported to LCAiT, an LCA software package (Step 3, Figure 2), to calculate the environmental impacts of the system using LCAiT databases. Finally, the impact assessment graphs together with the Life Cycle Inventories were exported to Excel files for LCA results presentation (Step 4, Figure 2).

3 SCENARIOS

In this section, the different scenarios are outlined with assumptions and data sources (full in-data sets may be found in [5]). The base case scenario is discussed in detail, whereas the other scenarios are only discussed in terms of how they differ from the base case scenario (see Table 1). Each change is compared to the base case scenario in order to identify the most important factors for change in the system.

Table 1: Different scenarios modelled (ticked), or not (crossed).

	Wood waste feedstock	Waste plastics feedstock
Base case	✓	✓
Gasifier improvement	✗	✓
H2 addition	✓	✓
Base case with hydropower electricity	✓	✓
Base case with coal electricity	✓	✓
Transport of feedstock from another country	✓	✓
Transport of methanol to the MTO	✓	✓

3.1 Base case scenario

3.1.1 GASIFICATION TO CLEAN SYNGAS AND PRODUCTION OF METHANOL

As mentioned in Section 2, gasification requires different technological solutions for treatment of biomass and plastic waste. The gasifier type used for biomass feedstock is based on pressurized fluidised bed gasification [6], [4]. Gasification technologies using a two-step reactor, where the biomass is first pyrolysed with subsequent gasification, has also been proposed [7]. When the aim is to maximise the methanol output, a catalytic reformer is placed at the output of the gasifier to decrease the higher hydrocarbons (including tars) in the syngas and to increase the yield of H_2 and CO [4]. A high H_2 content is suitable for methanol production.

For gasification of waste plastics, a study by Future Energy [8] evaluated the possibility of gasifying plastic waste in an entrained flow gasifier based on Noell technology. The aim of the study was to produce a synthesis gas with a high calorific value, which can be further processes to methanol. The feasibility study looked at gasification of 1 million tons of plastic waste per year, which for practical reasons was broken down into three process trains. Data from this study was used in the base case scenario, selecting a gasifier with water slurry. A higher quality syngas could, however, be obtained by the use of oil slurry in the gasifier.

The composition of the raw syngas from the gasifier, for both biomass and plastic waste, is given in Table 2. Without tar cracking, the syngas quality of biomass is close to the syngas from plastic waste.

Table 2: Composition of synthesis gas out of the gasifier

Component	**Biomass** (From [4])		**Plastic waste** (From [8]	
	Raw gas [vol%]	Dry basis [vol%]	Raw gas [vol%]	Dry basis [vol%]
CO	25.83	32.68	20.61	37.19
CO_2	15.81	20.0	12.2	22.01
H_2	33.53	42.42	21.3	38.43
H_2O	20.97	0	44.58	0
CH_4	0.17	0.22	0	0
N_2	3.65	4.62	0.75	1.35
HCl	0	0	0.54	0.97
H_2S	0.0147	0.0186	0.02	0.04
COS	0.001	0.0013	0	0
NH_3+HCN	0.0279	0.0353	0	0
$H_2/(CO+CO_2)$	0.81	0.81	0.65	0.65

The raw product gas from the gasifier reacts with steam in the WGS to increase the H_2 content in the syngas. All numbers, mass and energy balance, are adjusted to the new mass flow and composition by use of the Aspen HYSYS model. The H_2/CO-ratio at the outlet of the gasifier is the same for the syngas-based on plastic and biomass; however, the mass flow differs.

After the WGS reactor, sulphur and CO_2 are removed before the syngas can be transformed to methanol. The gas cleaning section was also modelled in HYSYS by using a component splitter to establish the mass flows. The component-split fraction is used for both plastic waste and biomass.

The off-gas from the methanol plant is combusted to generate steam. The methanol production in Figure 1 differs from plants converting natural gas into methanol, since it does not include steam reforming of natural gas. In addition, the MTO plant tolerates crude methanol as input, which means that the separation of methanol and water in distillation columns is avoided. Since pure methanol is not needed in the MTO process, crude methanol with about 20-30% water may be used [9]. The energy consumed is therefore reduced to 2/3 of what it would have been for pure methanol production. Indeed, the energy reduction was calculated by using a HYSYS model for methanol production, which shows that approximately 1/3 of the energy is used in separation [5].

The energy need for each unit is then calculated based on the energy flows given in the literature. The processes involved in waste to methanol have been assumed to be integrated through a steam island as suggested in [4]. The gasifier has excess energy used to produce steam directly, whereas the off-gases in the methanol reactor are burned in a heat recovery steam generator (HRSG) to produce steam. It is not clear whether this integration is the optimum, but the recovery of off-gases and high temperature processes show at least some process integration.

3.1.2 METHANOL TO PLASTICS

The MTO unit studied is the UOP/Hydro patented MTO process. Crude methanol is used in the MTO reactor, giving a product distribution as shown in Table 3. Ethylene and propylene are products used as feedstock in the production of PP and HDPE, whereas butene is sold as a by-product. The remaining products, flue gas, are burned to provide energy for the process.

Table 3: Product distribution from the MTO process [10]

Component		Product gas [wt%]
Products	Ethylene	55.2
	Propylene	27.0
	Butene	7.8

Flue gas	CO	0.32
	H_2	0.26
	CH_4	1.7
	C_2H_6	1.7
	C_2H_4	0.28
	C_3H_8	1.5
	C_4H_{10}	1.4
	C_{5+}	3.0

Using the product distribution from Table 3, the following are required to produce each kg of ethylene,: 3.74 kg methanol, 3.08 kg steam at 100 bars and 0.034 kWh electricity [10].

Plastic production is done using Borealis's Borstar technology [11]. The production of polyolefins is very clean and emissions originate mainly in the electricity production. The efficiency of ethylene to HDPE and propylene to PP is 100% and 98.7%, respectively.

The methanol-to-plastics is not integrated with the waste-to-methanol island. Process integration strategies could lead to better efficiency but are not considered in this paper. In terms of total steam balance, it is assumed that there is enough steam for all process steps when the off-gases from methanol and MTO are burned.

3.1.3 TRANSPORTATION AND ELECTRICITY

The transport of waste and intermediate products are included in the assessment. For the base case, feedstock logistics have only been modelled with the transport of woody biomass and waste plastics by trucks to the plant. For plastic waste, based on literature data from waste management [12], transport by truck for 200 km with empty return is used, and for wood, transport by truck for 123 km is selected (LCAiT Basic Tutorial Example: paper bag, 2001). The fuel used in transportation is based on fossil resources.

The electricity consumed in the production is assumed to be in line with the E.U. average, including a 9% grid loss. Changes in the electricity mix are discussed in Section 6.5.

The next section covers a description of the other scenarios and process configurations (Table 1).

3.2 Technological improvement of the gasifier

The gasification technology applied in the base case for plastic waste uses water slurry. The quality of the syngas from gasification of plastic waste can be improved by using oil slurry instead. In some cases, the slurry can be based on used oil. Used oil is not allowed on landfill sites and so one treatment method is to gasify it for energy or material purposes. When oil slurry is used, the calorific value of the feed to the gasifier increases, resulting in a higher quality syngas. Higher quality means less CO_2 and more CO and H_2 compared to the base case with water slurry.

The assumptions used in this scenario are:

1. Since the production of plastic waste is not included in the base case scenario, production and transport of the used oil is not included either. However, the overall impact of the transport can be assumed to be very low in comparison to other activities in the system.
2. The CO_2 emissions that directly come from the carbon atoms in the oil are accounted as “renewable” in order to be able to track down the carbon efficiency from the feed as it is done for plastic waste. “Non-renewable” is used for electricity and natural gas production.
3. The energy use for each process step is scaled with respect to the change in mass flows.

For biomass gasification, an improved technology is already used in the base case scenario with the inclusion of the tar cracker, and so no additional improvement was modelled.

Indeed, the performance of the modeled gasification technology is already in line with other [13],[14], who have evaluated technologies for the production of methanol from biomass that are likely to be commercial on the short term. They have shown that methanol can be produced from biomass with a net high heating value (HHV) energy efficiency between 54 and 58%. The scale of production was fixed at 400 MWth. Various process routes from biomass to methanol by use of the Aspen+ software have been modelled [15]. The objective was to identify concepts for biomass to methanol and hydrogen that may lead to higher overall energy efficiencies and lower costs on longer term. They have found that methanol can be produced from biomass with a HHV efficiency of 52-59%, confirming the statement here above. The corresponding HHV efficiency for the base case system described in Section 3.1 is 53.8%.

3.3 Addition of hydrogen

Another way to improve the system is to avoid the shift reactor through the addition of hydrogen to the system. Hydrogen is added to the syngas prior to the methanol reactor in order to adjust the H_2/CO-ratio in favour of the methanol production unit.

Hydrogen is produced both as a main product and as a valuable by-product in industrial processes [16]. The most widely used production route for hydrogen is the catalytic steam reforming of natural gas. When this technology is used, 50% of the hydrogen produced comes from water (steam) and 50% from the methane used as feed [16]. Another production route for hydrogen is the gasification of coal with downstream water gas shift of the carbon-rich synthesis gas. Hydrogen is also produced by the electrolysis of water.

This process requires large amounts of electricity, whereas all the hydrogen produced comes from the renewable resource of water.

Hydrogen is also an important by-product in a number of chemical processes. These processes include the production of chlorine from the electrolytic chlor-alkali process, crude oil refinery processes, the production of coke from coal in the coke oven gases and in chemical dehydrogenation processes such as ethylene plant purge gases, ammonia dissociation and hydrodealkylation [16]. In this study, it is assumed that by-product hydrogen from chlor-alkali and refinery processes was used. None of the emissions from the chlor-alkali or refinery processes are allocated to the hydrogen added, as it is seen as available as a by-product in excess.

Compared to the base case scenario, the WGS reactor is removed. Hydrogen is added to the syngas until the same H_2/CO-ratio as in the base case is obtained. All downstream units are adjusted linearly to the new mass flow.

3.4 Changes in electricity and transport systems

The electricity mix used in the base case scenario is the E.U. electricity mix, which is an average for electricity production in the E.U. However, other electricity mixes can be found, such as hydropower in Norway and coal-based electricity in some Eastern European countries. The change in overall CO_2 emissions with a change in electricity mix is shown in Section 4.

The transport of feedstock, intermediates and products all influence the overall global warming potential of the system. In the base case scenario, only the transport of the waste material is included in the results, since the processes are assumed to be located in the same place. In order to look at the influence transport distances have on the overall impact, increased transport distance for the waste material and transport of the intermediate product – methanol - is introduced (Figure 3).

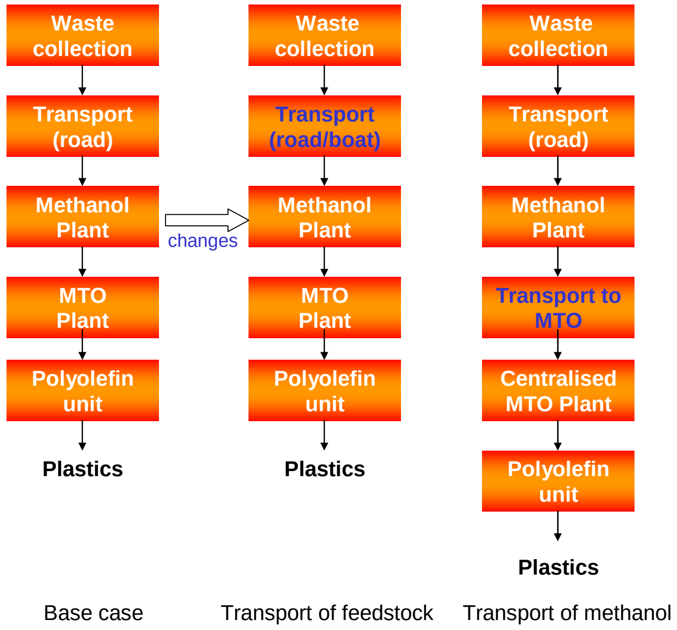

Figure 3: Changes in transport system

An example of the typical distance between a methanol plant based on natural gas and an end market would be from Santiago in Chile to San Francisco in California, a distance of about 9548 km. For the model in this study, 10000 km was selected, which represents the distance between the waste-to-methanol plant and the methanol-to-plastic plant. It is the distance between the region where the feedstock is available and where the waste handling facilities and infrastructures are neither developed nor greatly needed, such as south-east Asia or India, and Europe where the olefins conversion and high quality plastic facilities exist near the market (the distance between Singapore and Oslo, for example, is about 17000 km).

For the feedstocks, the transport distance is increased to the distance from Norway to Poland (Oslo-Gdansk). Therefore the overall distance becomes; transportation through Norway by truck of 123 km for wood wastes and 200 km for plastics, followed by 780 km by boat from Norway to Poland and finally, 300 km by truck in Poland, followed by an empty return.

4 RESULTS

The results are presented and discussed in a similar fashion to the way the scenarios were introduced in section 3 (Table 1). Only the CO_2 equivalents are presented here. More detailed results may be found in previous reports [5].

The results have one thing in common; the renewable CO_2 equivalents dominate (cf. Figures 4, 5, 6, 7, 8). The renewable CO_2 is defined as CO_2 from the waste material; the non-renewable CO_2 is derived from the production of electricity and use of fossil fuels for processes and transportation.

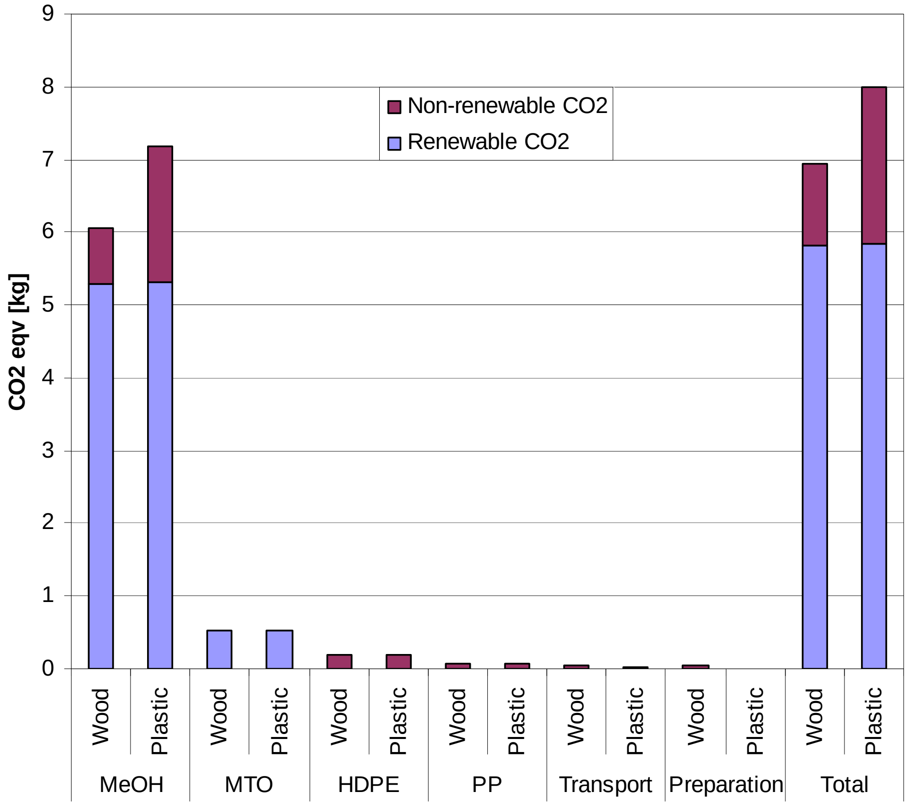

Figure 4: The global warming potential for each process step per f.u. kg polymer for the base case scenario.

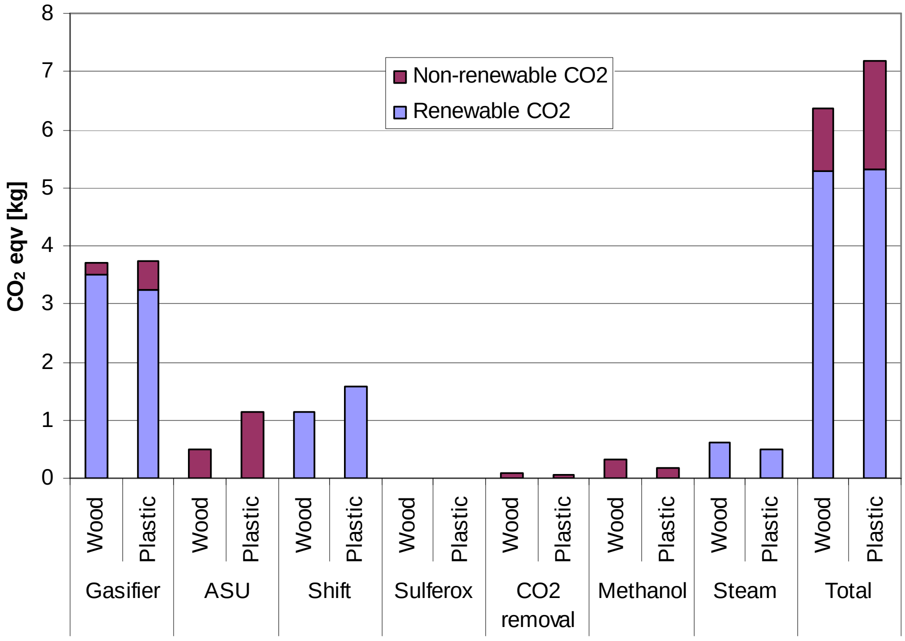

Figure 5: The global warming potential for each process step in production of methanol from waste per f.u, kg polymer for the base case scenario.

The main difference between the BTP and PTP is the large oxygen use in the plastic gasifier compared to the one used for biomass. There are two reasons for this. Firstly, and most importantly, oxygen content is higher in the biomass than in plastic waste (38.6 wt% compared with 7.1 wt%), which means that less added oxygen is needed for biomass. The second reason is the higher quality of the syngas from the biomass gasifier (lower CO_2 content), which means that less oxygen is needed to produce the unwanted CO_2 and H_2O. Moreover, to avoid dioxin formation, the product gas from the plastics gasifier is led to a direct quench, resulting in less high-temperature heat being available for steam generation.

The need for more oxygen in the plastic waste gasifier means that more oxygen has to be produced in the energy intensive air separation unit (ASU), which results in larger non-renewable CO_2 emissions (Figure 5). The other general trends that can be seen from the base case scenario are that electricity production dominates the non-renewable CO_2 emissions, and the methanol island (waste to methanol) is the dominant source for both renewable and non-renewable CO_2 for both systems.

Within the methanol island, the largest contributors are the gasifier, steam generation and shift reactor (Figure 5). The steam generation uses off-gases from the methanol reactor, and the combustion of this gas results in CO_2, which is assigned to the steam unit. The steam is used for all processes within the methanol island. The shift reactor shifts CO and H_2O to CO_2 and H_2, which results in renewable CO_2 emissions. The CO_2 emissions from the shift reactor can be reduced and even avoided by the addition of hydrogen or by having higher hydrogen content in the waste material. Improving the technology to decrease the CO_2 content in the syngas can reduce the renewable emissions from the gasifier. The non-renewable CO_2 associated with the gasifier can be decreased either by decreased use of oxygen, or a more energy efficient production than with an electricity-driven Air Separation Unit (ASU).

Improvement of gasifier

The biomass gasifier has a tar cracker at the outlet of the reactor in order to increase the yield. The plastic waste gasifier uses another technology, but a tar cracker could possibly also be useful for this configuration. By using oil slurry instead of the water slurry, the syngas quality is increased and the use of oxygen decreased. The result is less plastic waste feedstock being required for production of the functional unit, which then gives lower CO_2 emissions from the system (Figure 6). The decrease is 25 % and 35 % for renewable and non-renewable CO_2, respectively (see Table 4). The large decrease in non-renewable CO_2 equivalents is due to less oxygen being needed, whereas the decrease in renewable CO_2 equivalents is due to the higher quality of the syngas out of the gasifier (cf. Figure 7 vs. Figure 6). Neither transport nor production and use of the oil are included in the calculations above. For the transport of the oil, the figures will be close to the ones given for transport of waste. However, total Global Warming Potential (GWP) is not influenced largely by transport.

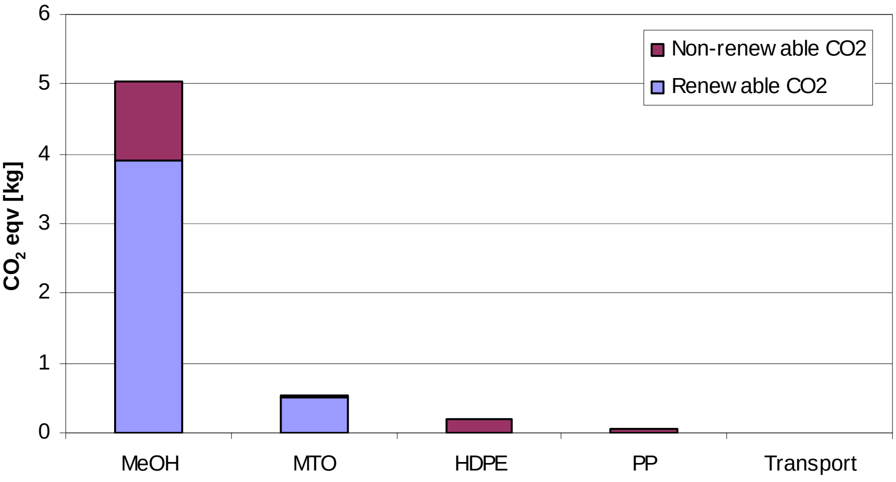

Figure 6: Global warming potential for each process step per f.u. kg polymer from waste plastics with oil slurry gasifier.

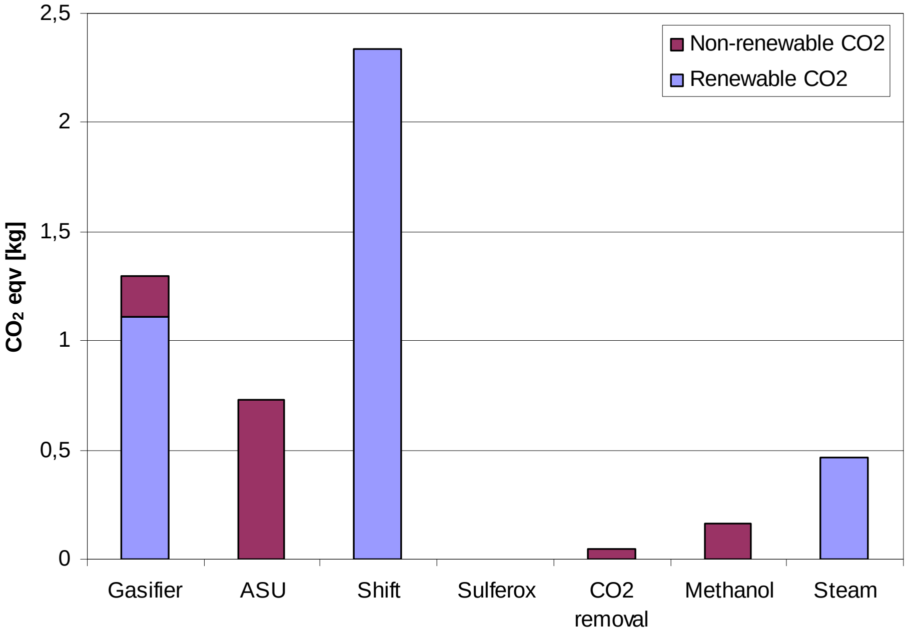

Figure 7: Global warming potential for each process step in the methanol island[1] per f.u., kg polymer from waste plastics with oil slurry gasifier.

[1] MeOH in Figure 4

Table 4: Summary of kg CO_2-equivalent (CO_2-eqv) and waste per functional unit for the various scenarios.

Scenario		**Renewable CO_2-eqv**	**Non-renewable CO_2-eqv**	**Waste per functional unit**	
				Dry	**As received**
Base case	BTP	5.8	1.4	4.7	9.4
	PTP	5.8	2.2	3.6	3.6
Improved gasifier	PTP	4.4	1.4	2.8	2.8 (1.4)[1]
H_2 added	BTP	3.5	1.1	3.4	6.7
	PTP	3.5	1.7	2.7	2.7

Hydrogen addition

Table 4 summarises the results for both plastic waste and wood waste. Compared to the base case, additional hydrogen improves the overall performance of both systems. Instead of shifting part of the CO to hydrogen, hydrogen is added to the high CO-content stream resulting in a higher plastic production. Higher plastic production means less electricity needed per functional unit, resulting in lower non-renewable CO_2 emitted from the ASU.

Renewable CO_2 is also reduced with this approach; the avoided shift reaction is the main reason for the improvement[2].

Electricity production and transport

In the base case scenario, the results indicate that transport is of minor importance (Figure 8), whereas use of electricity dominates the non-renewable CO_2 emissions. The choice of electricity mix in the base case is the E.U electricity mix. To examine the influence of electricity production, two extremes were tested: coal-based electricity and hydropower (see Table 5). Use of coal-based electricity increased the non-renewable CO_2 emissions almost 100%. The use of hydropower for all electricity production decreases the electricity-dependent, non-renewable CO_2 to close to zero, leaving the total non-renewable CO_2 emissions to be dominated by the emissions from transport. Since electricity dominates the non-renewable CO_2 emissions, choosing a low impact electricity production is of major importance.

Table 5: Change in total and electricity related non-renewable CO_2 equivalents with varying electricity mix, per f.u., kg polymer.

Electricity mix	**Electricity CO_2-eqv [kg]**		**Total CO_2-eqv [kg]**	
	Wood	Plastic	Wood	Plastic
E.U mix (base case)	1.1	2.0	1.3	2.1
Coal based	2.1	3.6	2.3	3.7
Hydropower	0.002	0.003	0.13	0.07

In addition to hydropower, other low impact electricity sources include wind power, solar cells and the combustion of biomass. These alternatives are not investigated further in this report. Another alternative is the production of more steam in the system, which can then be used to power the compressors that currently use electricity. Naturally, this will decrease the amount of waste bound for the plastic end-product. Compared to other studies where all electricity is assumed to be based on renewable resources [17], the base case scenario shows a higher global warming potential.

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[2] Results are valid only for a hydrogen excess scenario where H_2 is available in excess or as a by-product. The conclusions would not be the same in case of dedicated H_2 production systems such as natural gas reforming (cf. [5]).

By increasing the transport distances, the impact of transport has on the overall non-renewable CO_2 increases (Figure 9). The transport distance for methanol is longer than for the feedstock, which explains the larger impact for the transport of methanol. The transport-related, non-renewable CO_2 for the case with increased waste transport is approximately 4 times larger than the base case. When the transport of methanol is introduced, the transport-related, non-renewable CO_2 is 15 times higher than the base case. However, since transport has a low contribution to the total of non-renewable CO_2, the increase in total non-renewable CO_2 is 10 % and 30 % for transport of waste and methanol, respectively. It is important to note that from the base case it is known that the non-renewable CO_2 accounts for only 20-30% of the total CO_2 equivalents emitted from the system. The relative increase in the total GWP is thus even lower than the increase in non-renewable CO_2 with 8 % and 7 %, respectively. The findings are in agreement with other studies[18], [19] and [12], which have concluded that transport is of minor importance in waste handling when compared to the overall system .

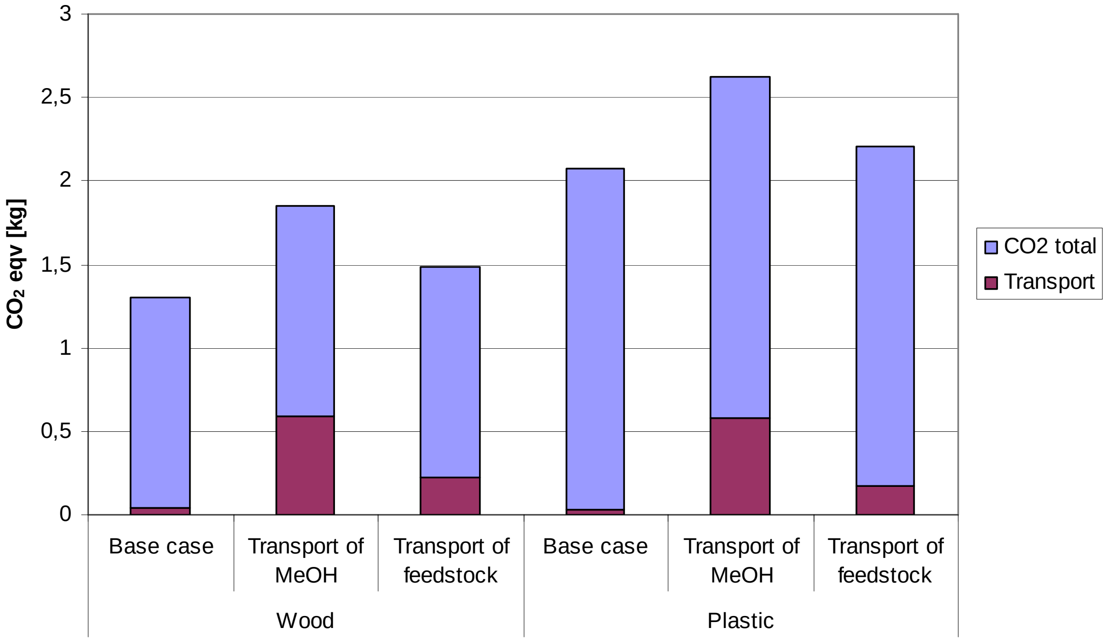

Figure 8: Change in non-renewable CO_2-eqv with increasing transport distances for methanol and feedstock, respectively per f.u., kg polymer.

5 *Discussion*

Hydrogen addition and CO_2 emissions

The CO_2 assigned to the shift reactor results from the shifting of CO to H_2 in order to increase the H_2/CO-ratio to the levels required in the methanol reactor. In one scenario, hydrogen was added to the system to avoid the shift reactor, and thereby reducing the CO_2 emitted from the system (Table 4). The additional hydrogen was taken as a by-product from chlorine production, refineries or similar, and consequently no environmental burdens were allocated to the hydrogen. With this approach, the reduction in renewable CO_2 was 40 % and non-renewable 22 % for both plastic and wood waste.

As discussed in Section 3.3, hydrogen can be produced from fossil fuels, water or renewable fuels like biomass. If a dedicated hydrogen production is used to produce the required hydrogen for the system, the environmental burden should be assigned to the system. The production of hydrogen from biomass gasification is the process route with lowest non-renewable CO_2 emissions [17]. It would be grotesque to build an additional biomass gasifier for hydrogen production in order to improve the performance of the existing gasification unit by avoiding the shift. It is possible to add a natural gas steam reformer to produce hydrogen rich syngas, where both the CO and H_2 in the syngas are utilized. The details of this approach are not discussed here. However, if hydrogen is available as a by-product from other processes, the improvement to the system is obvious.

"Biomass to plastics" and "plastics to plastics"

The most obvious difference between the systems with plastic and biomass waste is that the PTP process is a recycling system, whereas the BTP is an alternative production route to green plastics. This difference does not affect the technical performance of the system to a very great degree, however external conditions such as legislation, availability and marketing for the products might have an impact. These external conditions would in turn affect the technological choices for the system. An example could be the question concerning the addition of hydrogen, which might not make sense for biomass, unless hydrogen comes from a renewable resource. For plastic waste, the addition of hydrogen from a fossil resource is probably more logical when plastic waste is also based on fossil resources.

Waste monetization strategies and impact on the models

Raw, woody biomass waste has a high water content (~50%), so larger amounts of material – compared to waste plastics, coal, etc… - are needed to produce the same amount of methanol. Transport is of minor importance, but for long transport distances, the large amounts of water that is transported can be considered a disadvantage. Drying, pelletizing or even pyrolysis biomass waste before transportation could be an option. A decentralised-centralised model with a biomass/waste refining step between the collection and handling, and the fuel production step, could be interesting to study in the case of bigger feedstock amount use.

Environmental impact, positioning

For the BTP process, the Green House Gases (GHG) emissions - cradle to factory gate - are about 1.4 kg CO_2-eqv/kg plastic produced. Compared to production of various other polymers [22], this leads to the positioning given in Figure 9.

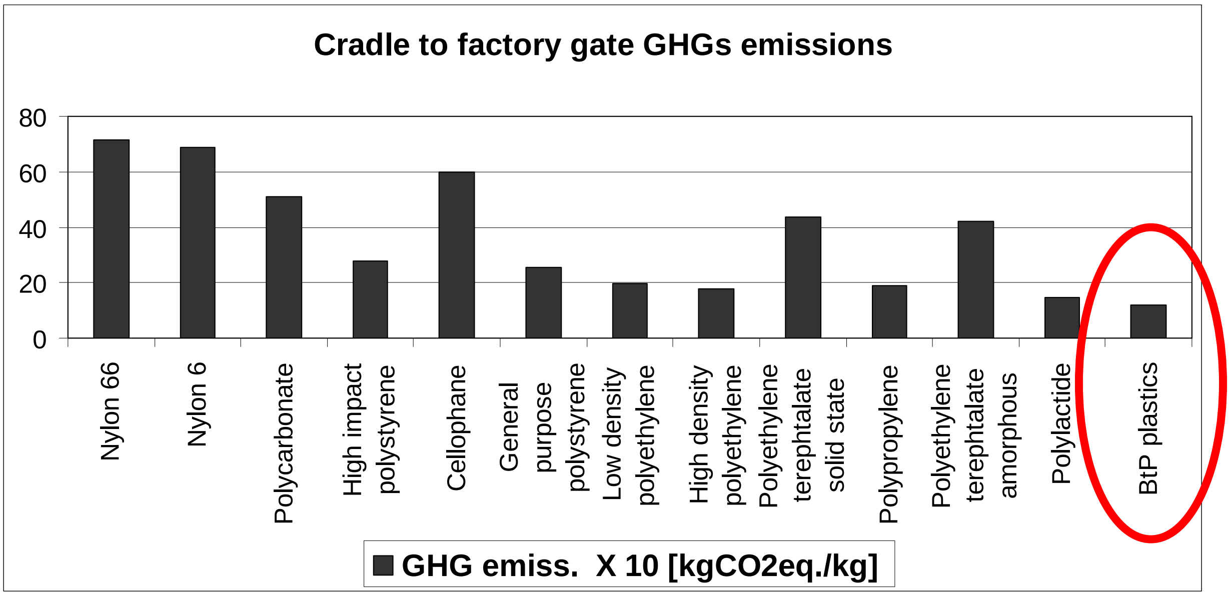

Figure 9: Comparison of plastic production from BTP with virgin production of various products.

The comparison of BTP and PTP is a little bit awkward, since the processes are more complementary than competing: the BTP process is a way to produce plastics from biomass thereby being an alternative to other plastics production processes, whereas the PTP in addition is an alternative to the management of plastic wastes and recycling, and could therefore be used to handle the plastics produced via the BTP at their end-of-life. From this perspective, using the term of “renewable CO_2” for the PTP process is very meaningful. Table 6 presents a comparison between the PTP and other plastic waste management systems. It shows that PTP could be an alternative to incineration or to recycling when plastic sorting systems are not very precise.

Table 6: PTP and plastic waste handling options

Direction	***Incineration (thermal energy plant)****	***Incineration Thermal energy and electricity****	***PTP***	***Recycling ”mechanical”***
Input	1 kg PE	1 kg PE	1 kg plastics	1 kg PE
Input			3.8 MJe	2.98 MJe

Output	3.14 kg CO2eq	2.44 kg CO2eq	2.2 kg CO2eq	0.15 kg PE residue
Output	43 MJth	25.3 MJth 11.5 MJe	0.27 kg plastics 68% HDPE 32% PP	0.85 kg PE

* spine@cpm database 2006 (MJe = MJ electricity and MJth = MJ thermal) [20]

** Tillman, Baumann 2004 [21]

6 CONCLUSIONS

Production of plastics from biomass and plastic waste appears to be technically possible using the BTP and PTP process routes. However, since these technologies are emerging ones, there are still many options regarding to their exact configuration. Several of these were investigated and were shown to be improvements from an environmental perspective. Optimizing gasification is of greatest importance, since the gasifier with its oxygen need is the main source of CO_2 emissions.

Sensitivity analyses were also carried out with respect to transport systems and the electricity mix. If coal-based electricity is used in the calculations, the total non-renewable CO_2 emissions increases by 75%, whereas calculations with hydropower results in a decrease of 90%. It was also shown that transport is of minor importance, although its contribution obviously increases as transport distances lengthen.

Both BTP and PTP show interesting possibilities compared to both virgin production and other recovery options. The environmental positioning of the BTP, outperforming both bioplastics and oil-based polymers, is confirmed. Moreover, the potential use of sources of excess hydrogen for purposes other than fuel-cell dedicated programs, like improving bioproducts production, is conclusive. The PTP process is closing the loop of plastic materials by a flexible recycling concept, since with a minimum need for pre-treatment like sorting and washing, both bioplastic and fossil fuel based plastics are potential feedstocks.

Finally, the method used for evaluating the concepts combines both process modelling and life cycle assessment. This gives a good understanding of the hot spots in the process with regard to both environmental impacts and process performance. The method also enables an effective early-design phase evaluation.

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Making technology screening usable for environmental assessment: the case of biopolymers

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Abstract

Directly applying information obtained from technology screening in environmental assessment methods, such as Life Cycle Assessment (LCA), could lead to severe deficiencies, such as inconsistencies or the omission of important alternatives. It is indeed difficult, especially in the case of emerging technologies, to know whether or not the technology is ready for adoption, what its underlying assumptions are, and whether it fits the LCA goal and scope definition. It is thus easy to make mistakes that could jeopardize the coherence of an environmental assessment. This paper presents a method for preventing such mistakes and helping gauge and map information obtained from technology screenings, for use in environmental assessments such as LCA. The method is based on a series of steps that help organize information in a bottom–up way. Information as diverse as technology status and fashion will be mapped and gauged for our specific case study: bioplastics production. When the method is applied to the case of bioplastics, common mistakes such as anachronisms within the LCA time horizon or omitting essential processes, such as syngas-based ones, are greatly reduced. Moreover, the method ensures a background of information maps and data that can be further used when conducting LCA derivations and formulating “what-if” scenarios.

Keywords: technology screening, LCA, bioplastics, time horizon, goal and scope definition.

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1 Introduction

New technologies are often characterized by uncertainties, high risks, and huge investments. To reduce the risks, screening the technology of an emerging field is a common first step preceding engineering projects. If we are dealing with sustainable innovation, this step is often followed by environmental assessments.

In terms of materials, an environmental assessment presupposes that a process route has been identified. This process route should be coherent in terms of time horizon and technological maturity, and “solid” enough in terms of available emissions/energy data.

However, the technology screening literature[1] [2] [3] [4] reveals that there are a number of limitations in terms of how information from technology screenings has been used in conducting environmental assessments, such as LCA. These limitations refer to a set of methodological weaknesses; for example, data regarding technologies both currently and yet to be applied in industry are unjustifiably mixed, the pilot plant and demo unit status of some technologies are not highlighted, and integration with other industrial sectors is not indexed. The uncritical use of concepts from the existing screening literature may thus lead to environmental assessments that are based on information that could produce misleading and irrelevant results. This paper presents a method that avoids such weaknesses, making technology screening a more useful basis for the environmental assessment of emerging technologies. This could fill a gap in the ISO 14041 standard, which does not state that the choice of technology to be assessed or what options to study is an issue;[5] moreover it could also help in formulating coherent scenarios in LCA studies.[6]

The paper is structured as follows. In the next section, the weaknesses uncovered in some of the technology screening literature are discussed in more detail. Section 3 presents a method for overcoming such weaknesses. The method will be presented as a set of steps; for illustrative purposes, each step will be applied to the bioplastics case. Section 4 compares an LCA using conventional technology screening and the same LCA using our method. Section 5 presents the main conclusions.

2 Weaknesses of using technology screening information in environmental assessment

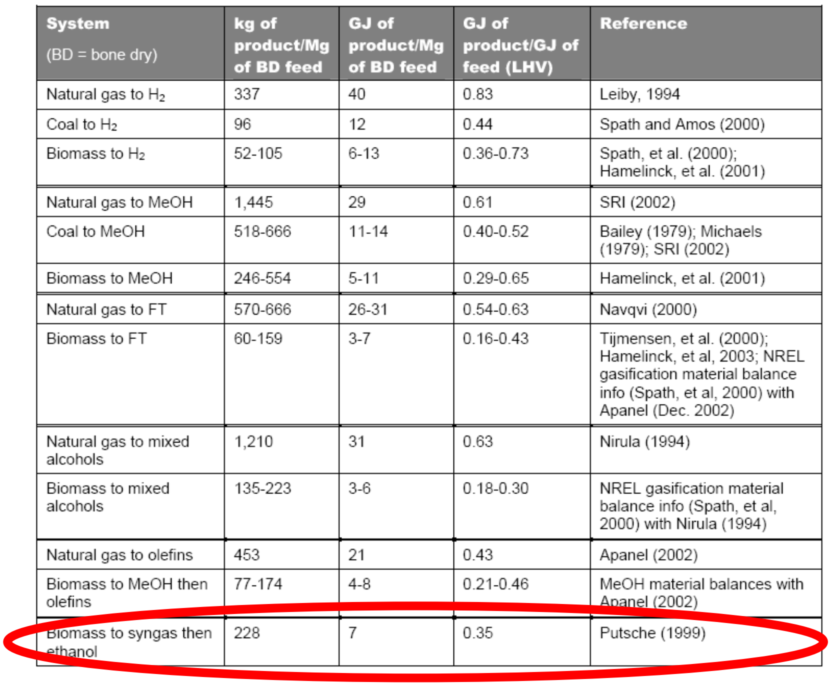
Most technology screening reports are not intended for direct use in environmental assessments, so when they are used uncritically for this purpose, flawed assessments may result. These screening reports present a wealth of information that needs to be appropriately “organized” to be used for such assessments. Moreover, due to their inherent context, the reports may “miss” some information that is relevant to environmental assessment. Let us explain what we mean by “organized” or “missing” information and the consequences for environmental assessments.

The information that needs to be “organized” is information that is mixed and not gauged. In technology screening reports, a range of information pertaining to all types of technologies is often mixed; for example, a clearly defined time horizon may be lacking (i.e., current technologies, technologies to be applied in the near future, and very “futuristic” technologies are mixed in the screening) or information stemming from very different organizational backgrounds may be mixed (e.g., information from academic, industrial, and military sources). It is thus easy to mix incompatible technologies when conducting an environmental assessment based on such information.

For example, a technology screening may present a panel of technologies without mentioning the technology status or time horizon or any of them, since the focus is perhaps on other issues. The consequence of directly using data from such a technology screening for an environmental assessment, such as an LCA, could well be inconsistent results. The technology screening data would be incompatible with the goal and scope definition that clearly states, for example, that the technologies assessed must be coherent with a particular time horizon.

For example, table 1 indicates the yields and energy efficiencies of various chemical processes used in producing alternative fuels.

Table 1: **Feedstock to Product Material Balance Information** [1]



System (BD = bone dry)	**kg of product/Mg of BD feed**	**GJ of product/Mg of BD feed**	**GJ of product/GJ of feed (LHV)**	**Reference**
Natural gas to H_2	337	40	0.83	Leiby, 1994
Coal to H_2	96	12	0.44	Spath and Amos (2000)
Biomass to H_2	52-105	6-13	0.36-0.73	Spath, et al. (2000); Hamelinck, et al. (2001)
Natural gas to MeOH	1,445	29	0.61	SRI (2002)
Coal to MeOH	518-666	11-14	0.40-0.52	Bailey (1979); Michaels (1979); SRI (2002)
Biomass to MeOH	246-554	5-11	0.29-0.65	Hamelinck, et al. (2001)
Natural gas to FT	570-666	26-31	0.54-0.63	Navqvi (2000)
Biomass to FT	60-159	3-7	0.16-0.43	Tijmensen, et al. (2000); Hamelinck, et al, 2003; NREL gasification material balance info (Spath, et al, 2000) with Apanel (Dec. 2002)
Natural gas to mixed alcohols	1,210	31	0.63	Nirula (1994)
Biomass to mixed alcohols	135-223	3-6	0.18-0.30	NREL gasification material balance info (Spath, et al, 2000) with Nirula (1994)
Natural gas to olefins	453	21	0.43	Apanel (2002)
Biomass to MeOH then olefins	77-174	4-8	0.21-0.46	MeOH material balances with Apanel (2002)
Biomass to syngas then ethanol	228	7	0.35	Putsche (1999)

Anachronism no warning

If data from the above table were used directly in an environmental assessment to calculate the total energy used in producing the different products, the results would describe the environmental performance of 12 technologies that have been *industrially* experimented with (the 12 first in the table) and that of one (the 13th and final technology) that has only been tested in certain advanced laboratories. In terms of technology status, the last technology does not fit into the same time horizon, so the comparison is not particularly meaningful. Because the information, in this case regarding technological maturity, has not been properly organized and gauged, comparing the last technology with the 12 previous ones is hardly relevant for an environmental assessment. A reasonable reader would ask, “Why is this technology included, since it can be implemented only on a completely different time horizon?” Or, “If this 13th technology is included, why were other equivalently “futuristic” technologies not included?” These are justifiable questions that raise serious doubts about the coherence of such an assessment, doubts that the method presented in this paper sets out to handle.

As mentioned above, time horizon differences are not the only matters that may be poorly handled; geographical and other information, for example, may also be vague or omitted, leading to incoherent or irrelevant results. Organizing such information properly will ensure that any environmental assessment based on it is coherent. By gauging information, for example, in terms of the maturity, potential, and expectations of the technologies dealt with, environmental assessments will deal with a pool of comparable technologies, each of which is included in the assessment for justifiable reasons. Using this method, each of the technologies will have been environmentally assessed for good reason, and we will avoid cases like that in table 1, in which one of the presented technologies clearly does not fit, at least in terms of technological maturity status.

“Missing” information is another classic problem when technology screening is used for environmental assessments. Indeed, the context of the technology screening could well lead to the selection of a pool of similar technologies (e.g., white biotechnologies),[I] thereby missing other technologies that are highly relevant for the purposes of an environmental assessment. A good example of such a “missing” technology is provided by the last IPTS report on bio-based polymers.[4] To produce biomaterials (e.g., fuels, chemicals, and polymers), there are basically two types of technologies: white biotechnologies and thermochemical technologies. Both these types have already been considered and environmentally assessed for alternative fuel production (Edwards et al, 2003); however, the last E.U.’s Institute for Prospective Technological Studies (IPTS) report, because it did not “organize” information regarding the polymer precursors (e.g., signs of “take-off,” industrial integration, and expectations), simply overlooks the thermochemical processes, leading to an incomplete environmental assessment: it overlooks half the available technologies for producing biomaterials.

I will now present a method that helps us avoid such mistakes, making technology screening information “safer” for use in environmental assessments.

3 Method presentation and application to a “biomass-to-plastics” case study

This method allows technology screening to be used as a basis for environmental assessments, such as LCA, while avoiding the problems discussed above. To achieve this, a mapping procedure is suggested to decrease the risk of “missing” vital factors, and information will be gauged so it can be properly “organized” and taken into account when constructing scenarios for environmental assessment. This method will ensure that within the pool of environmentally assessed technologies, all are included for coherent reasons; this will prevent misleading comparisons, like the one presented in section 2, concerning technology status. The method comprises six steps and can be characterized as a bottom–up strategy. We start by mapping and gauging elementary structures (molecules) and end with complex ones (industrial networks); we move from objects to subjects, from technological maturity to public expectations. This ensures an objective vision.[II]

Each step will either have a mapping purpose—not to miss anything—or an “information organizing” purpose, so as to evaluate and offer reasons why each production route should fit into a pool of routes to be environmentally assessed. The six steps of the method will first be briefly described in table 2, and then described in greater detail in the subsequent section, where the method is applied to a specific case for illustrative purposes.

Table 2: Six-step method for organizing information

Steps	What is done	Why is it done
Step 1	Define feedstock, products, and time horizon.	This step is fundamental to establishing the boundaries of what we are dealing with. It explains the basis on which any chemical intermediates may be

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[I] White biotechnology, also known as grey biotechnology, is biotechnology applied to industrial processes (for example, designing an organism to produce a useful chemical). (wikipedia.org).

[II] Applying a bottom–up strategy, we start by mapping and organizing information regarding objects (e.g., molecules and chemical reactions); this helps us maintain objectivity, since the organized information does not relate to entities, like companies or industrial sectors, that could be considered as subjects.

		selected.
Step 2	Map routes from feedstock to products.	This step helps reduce, from the outset, the risk of missing potential process routes.
Step 3	Gauge maturity of the technology.	This step organizes information concerning existing routes and distinguishes between routes of differing degrees of technological maturity (i.e., those already commercialized, soon to be commercialized, and still needing much more development).
Step 4	Assess technical activity levels.	This step helps organize information regarding the development intensity of processes in terms of volume of technological activities (e.g., patenting). It provides reasons for potentially including certain processes in an assessment.
Step 5	Gauge and map routes according to potential for integration with other sectors.	This step organizes information regarding the potential of some routes with respect to their integration with other sectors. The mapping helps identify intermediates having great potential for integration with other sectors; this provides arguments for cross-sector processes.
Step 6	Gauge public expectations.	This step organizes information in terms of expectations regarding certain routes. It provides reasons for considering fashionable processes.

For illustrative purposes, we chose to apply our method to bioplastics (in this case, plastics produced from biomass in Sweden and Western Europe). This is an appropriate case study due to its inherent complexity in terms of both technology and environmental expectations. This inevitably leads to many technology screenings and a huge demand for environmental assessments, such as LCA; the risk that technology screening results may be uncritically used for environmental assessment purposes is thus obvious.

Step 1: Define feedstock, products, and time horizon

In this first step, we clearly specify the process route we are going to study.

a. This process will convert the feedstock, F, into a final product, P, both of which must be clearly defined.[III] The physical and chemical properties of the feedstock and the final product will determine the types of processes and reactions that link one to the other. Since the environmental impacts depend greatly on the technology choice, it is necessary to have clear definitions of the feedstock, final products, and intermediates

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[III] Having a clear definition and the same level of detail regarding the different compounds studied is crucial, particularly in the case of the feedstock. Too many LCAs compare routes from oil, coal, and gas to routes from corn, sugar cane, and other very specific feedstocks. It is a huge mistake to consider oil to be a homogeneous compound like corn or sugar cane: in terms of atomic composition, there is as much difference between two types of oil as between sugar cane and corn. For reasons of coherence, the level of detail regarding the definition of all compounds studied should be approximately the same.

if we want to make a meaningful environmental assessment afterwards (see the LCA goal and scope definition in ISO 14041: section 5.3.3 p. 6).

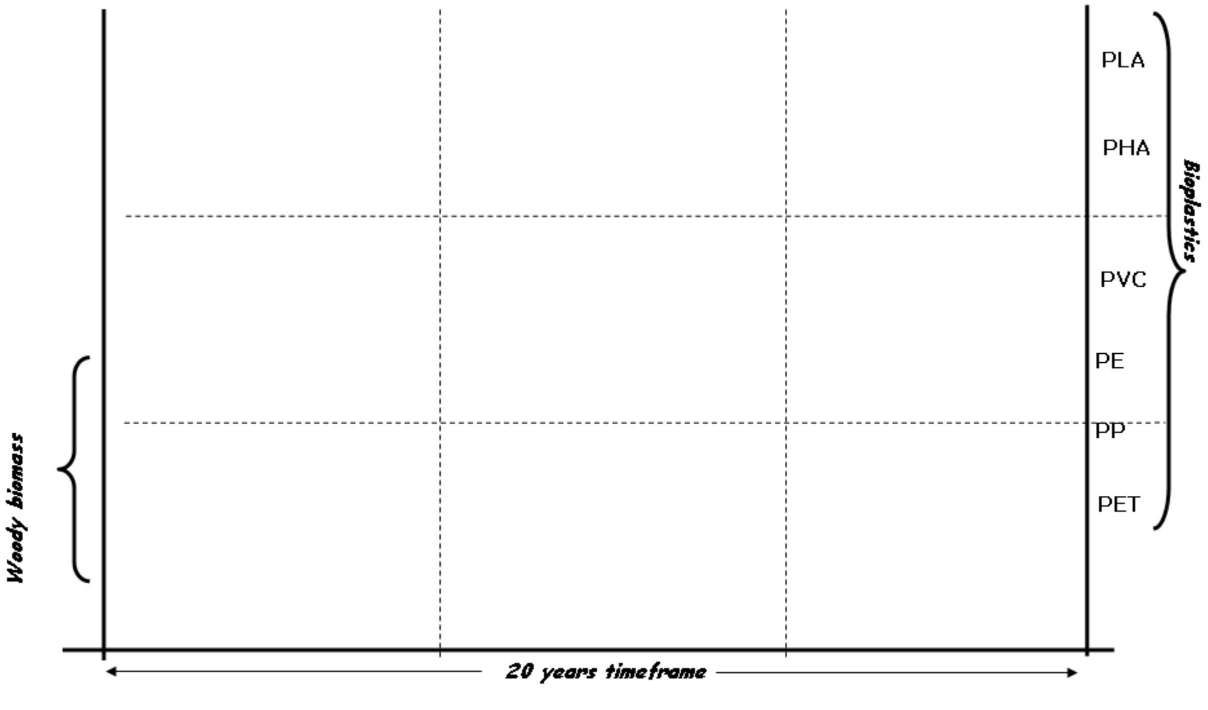
b. The time horizon also must be clearly defined and the technologies screened must be consistent with it (see section 2).

What has been described above in a. and b. in general terms will now be applied to bioplastics.

a. This process will transform biomass feedstock into plastic products. For regional reasons, we will focus on waste wood biomass, in which Sweden has a huge potential.[7] About the plastics, for simplicity reasons, we will consider only bioplastics with properties the same or superior[IV] to those of their fossil fuel-based counterparts. We focus on mass production (no small-production biopolymers, for example, for medical applications, will be considered), such as packaging applications, for obvious environmental reasons.

b. We will consider a time horizon of approximately 20 years (the usual time for petrochemical projects), i.e., one without radical changes in surrounding technologies. It is assumed that the electricity system will be based on roughly the same technologies as it is today (i.e., no fuel cell-based power plants, no lunar Helium-3 fuelling dedicated nuclear powered plants[8]) and that oil, gas, and coal will still be used extensively. The geographical boundaries we chose for the production facilities are those of Western Europe.

This sets the boundaries of the process routes we are about to identify and constitutes the first step of the method (see figure 1).



[IV] This means that thermoplastic starch (TPS), polyvinyl alcohol (PVOH), and other such bioplastics will not be considered, since their inherent properties are quite low compared to those of polyolefins. However, we do not see why specific applications of bioplastics (such as plastic bags and certain films) should require the properties as stringent as those of fossil fuel-based counterparts if the bioplastics can fulfill the same tasks. However, for the sake of simplicity and comprehensibility, the study will consider only biopolymers that are functionally equal or superior to their fossil fuel-based counterparts.

Figure 1: The boundaries and time horizon of the bioplastics case study are fixed. The feedstock, final products, and time horizon are all defined. All technologies or concepts within the boundaries (i.e., arrows) lie within a 20-year time horizon.

Step 2: Mapping potential production routes based on scientific and engineering data

The second step uses a “vice” procedure for identifying process routes, starting from both a feedstock and a product perspective. What processes can the feedstock feed and what processes can produce product P? After this, we look at the intermediates and products that can be made from the feedstock and at the building blocks can be used to make the final product; we then try to determine the available and potential bridges between them. This strategy is close to what chemists do when combining the synthesis and retrosynthesis perspectives.[V] Again, this vice procedure helps ensure that we do not miss anything.

Applying the vice procedure to bioplastics leads to two questions: 1) In what processes can wood waste be used? 2) What processes can produce plastics? In turn, we ask what chemical intermediates can be made from the biomass and from what building blocks can plastics be made. We can then identify the available and potential bridges between these chemicals. Thus, we build a map of all potential reactions and chemical intermediates between biomass and plastics (see figure 2).

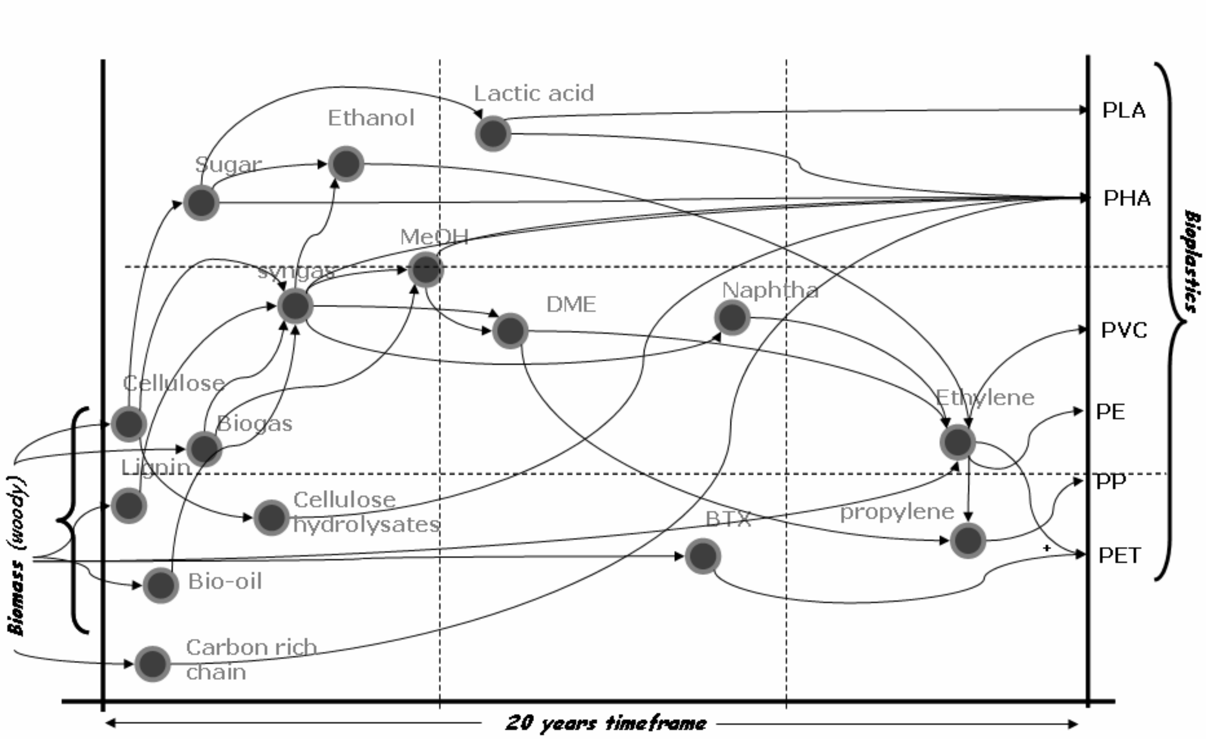


Figure 2: Mapping bioplastic processes and intermediate chemicals. Reactions are indicated by arrows and intermediates by dots.

[V] Retrosynthetic analysis is a technique for solving problems encountered when planning organic syntheses. It is done by transforming a target molecule into simpler precursor structures without making any assumptions regarding the starting materials. Each precursor material is examined using the same method; this procedure is repeated until simple or commercially available structures are reached. (wikipedia.org).

To make a coherent environmental assessment of a pool of technologies, one must assess and compare groups of potential processes that can only be identified by knowing the real potential of each route and intermediate in terms of research and industrial applications. The above mapping is not sufficient; we also need to gauge the different routes to avoid situations like those described in section 2, and for this we must know the different statuses of all the routes (e.g., technological maturity, public acceptance). That is what the following steps are for: they identify and organize information regarding the potential routes that could be environmentally assessed in further work.

Step 3: Gauging the technological maturity

When the links between the intermediates have been identified, we must specify the technological maturity of the links (e.g., R&D, pilot testing, and demo and industrial projects) in order to characterize the degrees of maturity of the various routes.

Applying the method to the bioplastics case study leads to the following steps. When the chemical reactions have been identified, we then analyze the technological status (theoretical, lab, pilot, commercial, etc.) of each reaction in order to determine the technological maturity of the various chemical routes mapped. Thus, the map (see figure 3) of all potential reactions and chemical intermediates between biomass and plastics is complemented with information regarding the actual maturity of the technology for each reaction.

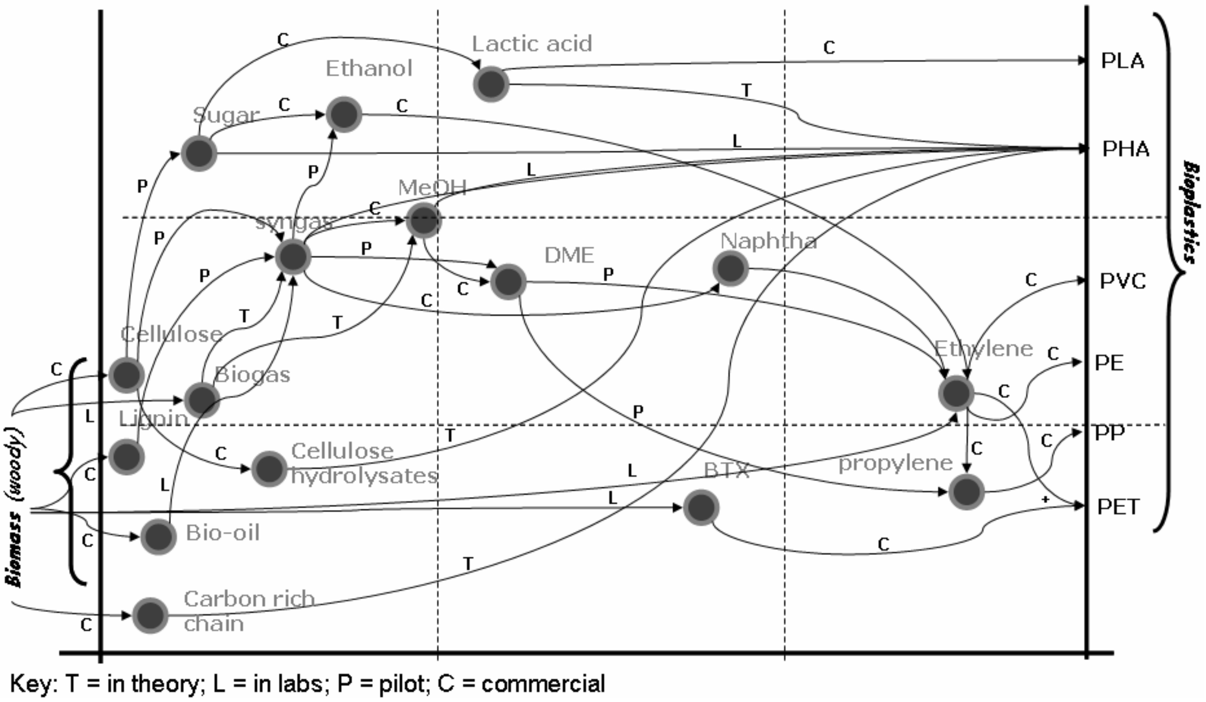


Figure 3: Bioplastics routes and intermediates with associated technological maturities.

Mapping provides important information concerning the technology statuses of the various reactions, thus allowing us to identify which routes currently exist and which are more "futuristic." It helps us in case we are asked why a particular technology has been environmentally assessed; that a given technology is mature and already developed is one of the answers.

However, a route that today largely has a “lab” status but that has been subjected to much R&D, or that runs through intermediates with highly industrial statuses, could be as important as a well-known technology route. The above mapping does not, therefore, prevent us from making errors arising from using unorganized information in an environmental assessment. Take, for example, 10 different processes, all of which use well-known technologies. If one with a “lab” status is to be environmentally assessed like the others, then its lab status should be supported by other criteria, such as considerable R&D activity or potential for great industrial integration. By organizing the information in this way, we can keep the environmental assessment coherent (see section 2). Again, the goal is to be able to state why a particular route has been environmentally assessed, by explaining, for example, that it is supported by considerably more R&D activity than other routes. That is what we will deal with in the next step.

Step 4: Technical activity gauging

To identify the routes with large potential (i.e., to organize information) using production route mapping, we gauge each link and intermediate according to the amount of related technical/industrial activity. This can be quantified, for example, by analyzing patents, industrial capital expenditure (CAPEX), and R&D spending. We propose an indicator that combines an *intensive* value, such as knowledge (e.g., patent analysis and R&D spending), and an *extensive* value, such as production volume or market size. Again, the purpose is to organize information and to find justification for assessing certain production routes, since some could have been underestimated or omitted if we had stopped at the previous step and conducted an LCA based only on the mapping, leading to erroneous results (see section 2).

Applying such gauging to the bioplastic case study involves assessing the market size of each intermediate using market price and production volumes, to give an idea of the industrial strength of each intermediate. Moreover, to assess the research activity connected with each intermediate, a patent number search was also performed (see Appendix 1).

Since the number of patents is assumed to be quite dependent on market size, we have calculated the number of patents in proportion to the market size for each intermediate. This indicator identifies those intermediates associated with high research activity compared to production, and may thus indicate the future development potential of the intermediate.

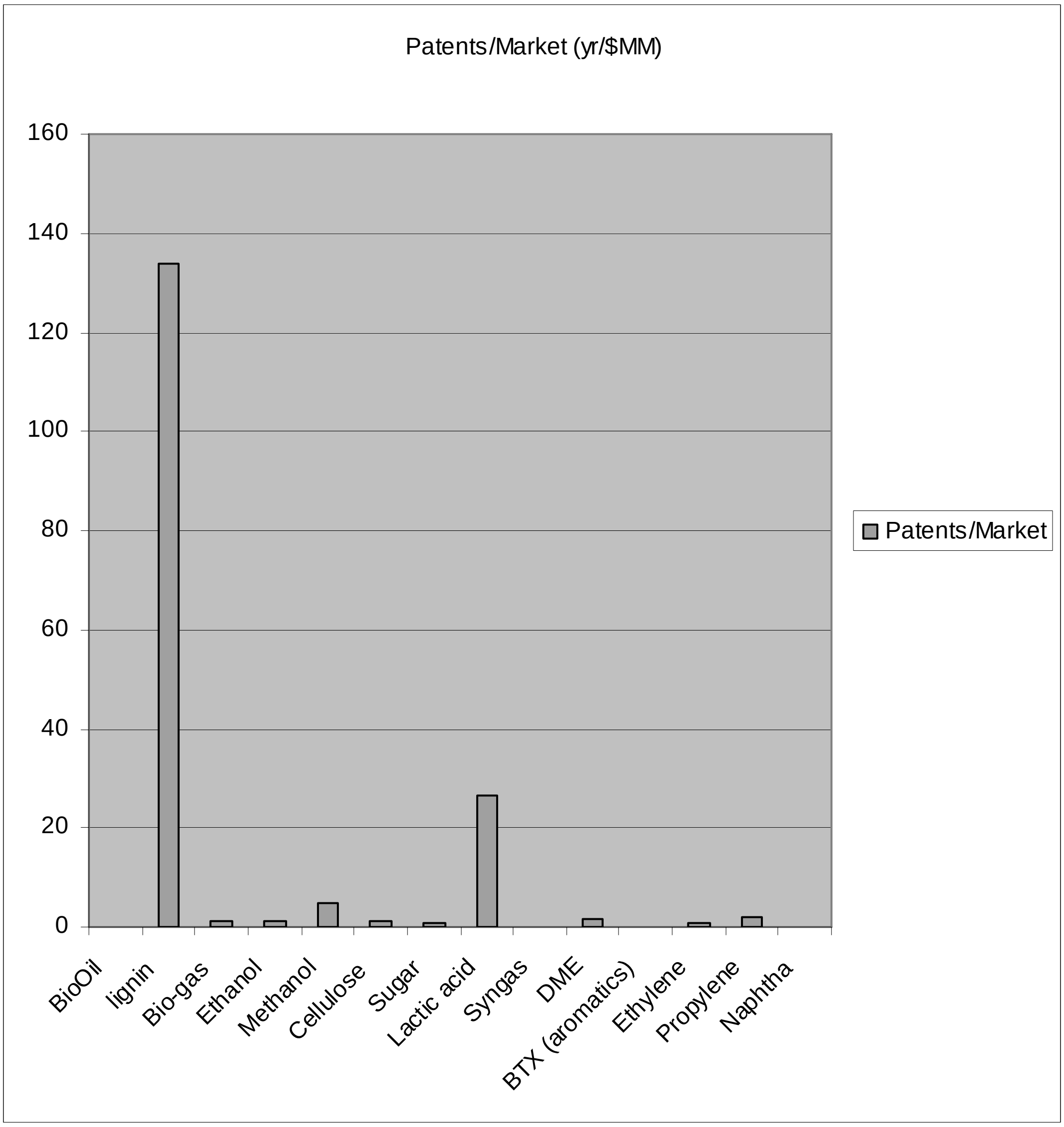


Figure 4: Total number of existing patents worldwide, normalized by market size, for each intermediate. The number of patents is the cumulative worldwide total from the year 1836 on. The results come from the esp@cenet quick search engine of the European Patent Office, using the intermediate's name as the entry word. The market size ($MM/year) is evaluated by multiplying the world production capacity (~2004) by the market price of each intermediate (obtained from ICIS website, www.icis.com).

The results (see figure 4) suggest that some intermediates have strong potential. Lignin is certainly in the spotlight, being associated with many patents and a small market. Lactic acid ranks second due to its many patents and medium production volume. Methanol, in third position, performs quite well despite its huge production, implying that the associated patents are quite numerous, due to new emerging applications (e.g., biodiesel, direct methanol fuel cells, and methanol to olefins). Some other intermediates, such as benzene, toluene, and xylene (BTX), have low potential compared to that of lactic acid, lignin, and methanol.

The routes using those high-potential intermediates are associated with considerable technical activity; hence, at a given technology status level, the routes going through those intermediates will be "favored," in that they will benefit from the technical activity associated with those intermediates. The routes going through high-potential intermediates are thus high-potential routes: though the technologies may not yet be of commercial status (unlike ethylene obtained from ethanol dehydration), there is a stronger likelihood that these routes will be highly relevant and hence should be subject to environmental assessment.

However, some intermediates may be on the verge of becoming important, due to more recent growth in technical activity. So as not to miss such intermediates, we refine the indicator by incorporating a patent search covering the past seven years (the previous indicator is based on cumulative patent counting). Knowing the progression in the cumulative number of patents over the past seven years for each intermediate can give an idea of the trend in knowledge development. Again, a patent progression analysis, in proportion to market size, has been performed to determine the strength of progression of some intermediates from 1999 to 2005.

Figure 5 presents the research activity trends for all intermediates in relation to market size. It indicates the inherent trend strength the last seven years for each intermediate, and helps us identify potentially important intermediates that we may not have noticed in the previous analysis. The three greatest increases in technical activity are associated with lactic acid, lignin, and DME.

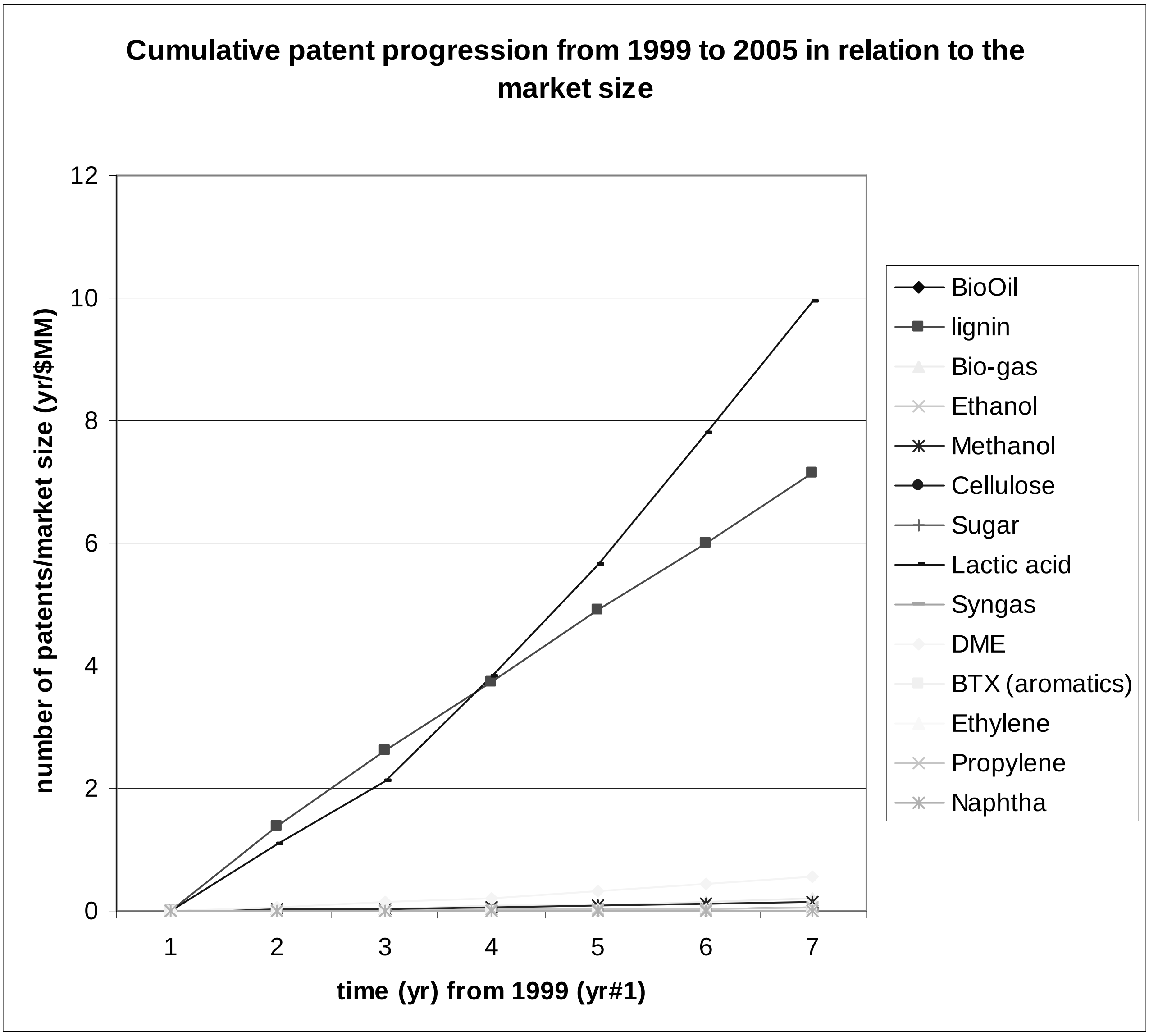
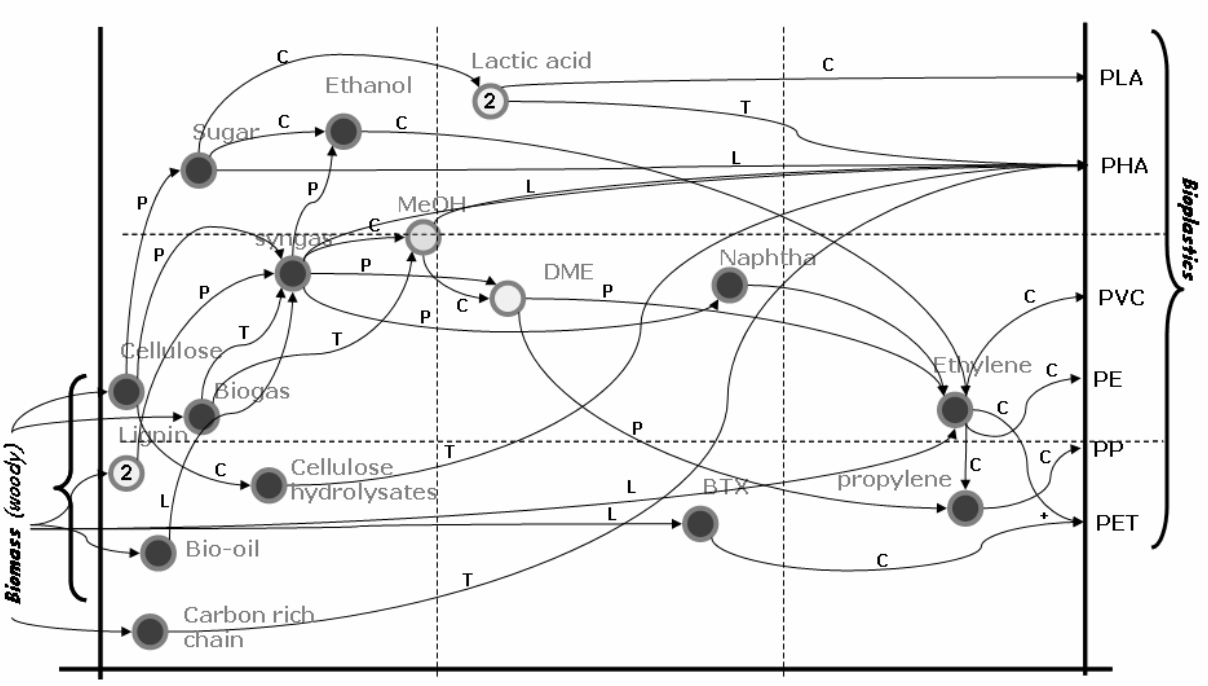


Figure 5: Patent trends normalized by market size for intermediates in potential bioplastics routes. The number of patents is cumulative worldwide by year and is obtained from the esp@cenet quick search engine of the European Patent Office, using the intermediate's name as the entry word. The market size ($MM/year) is for each intermediates occurring between biomass and bioplastics. The market size is evaluated by multiplying the world production capacity (~2004) by the market price (obtained from the ICIS website, www.icis.com).

Using this "patent dynamics indicator" (see figure 5) much the same pattern emerges, again indicating high-potential routes associated with intermediates with high "patent dynamics" over the last seven years (light dots). It is much the same pattern that emerges, even though in figure 5, lactic acid, lignin, and DME are the ones that emerge as favorites instead of lignin, lactic acid, and methanol in figure 4. However, DME is the dehydrated version of methanol ($2CH_3OH \rightarrow CH_3OCH_3 + H_2O$), and the DME market is one step ahead of the methanol one. Therefore, we will consider those two compounds to be very similar, and we could say that the pattern is approximately the same, even though it is DME instead of methanol that is associated with increasing research activity. These routes involve intermediates with high recent patent intensity growth, even though their technology status may not yet be ready for pilot testing or commercialization.



Key: T = in theory; L = in labs; P = pilot; C = commercial

Figure 6: Superimposing the gauging for "favored" intermediates using the technical activity gauging indicators (light grey dots). A number 2 in a light dot means that the intermediate has also been "favored" by a second indicator. Figure 6 is the result of superimposing the indicators depicted in figures 4 and 5.

Figure 6 displays the complete results of gauging the technical activity associated with each intermediate. The results of this gauging indicate that while some routes may not be commercially available, they may indirectly be associated with high technical activity because of the intermediates they go through. This would strongly justify including those routes in the pool of routes, leading to bioplastics, to be subjected to environmental assessment.

Step 5: Gauge and map routes integration

The next step is to assess the possible links of a route and its integration with other industrial sectors. The integration factor could influence or even counterbalance the preceding gauging, making one intermediate more attractive than another because of its relationships with a powerful and growing sector. The goal is here to identify routes/intermediates that may have low technical activity levels but highly developed links with other sectors. A high level of such integration will make a particular intermediate and route more relevant for environmental assessment. Again, the purpose is to avoid missing potentially important routes and to assess the various intermediates in order to have a coherent comparison when the screening is applied to environmental assessment. One way to map this integration is to look one step upstream (i.e., at possible production routes) and one step downstream (i.e., at primary potential applications) to see what and how many industrial sectors are involved.[VI]

Applying this "filter" to the bioplastics case study, we assess the links/integration of each intermediate with other industrial sectors. The integration of an intermediate can be quantified by examining the different feedstocks and pathways (i.e., industries) involved in producing it, and the different potential products and applications arising from it. The data used in this assessment are found in Appendix 2.

Table 3 presents the integration level of each intermediate, more stars indicating a more integrated intermediate.

Table 3 Level of integration of intermediates with downstream applications and upstream feedstocks[VII]

Cellulose	**Lignin**	**Bio-oil**	**Carbon Rich chain**	**Bio gas**	**Sugar**	**Syn gas**	**Cellulose hydrolasates**	**EtOH**	**MeOH**	**Lactic acid**	**DME**	**BTX**	**Naphtha**	**propylene**	**Ethylene**
***	******	*****	**	****	***	********	**	*******	********	*******	******	****	***	*******	***********

The three most integrated intermediates are syngas, ethylene, and methanol (see figure 7 where these are presented using light dots). The links with natural gas industries are very strong in the case of methanol/DME, syngas processes, ethylene, and propylene. The ability of these intermediates to be produced from both biomass and fossil fuels gives them a big advantage in terms of integration.

[VI] This also allows for the analysis of short-term potential (i.e., of growth potential). Indeed, white biotechnology intermediates (e.g., sugar from corn, lactic acid) profit from integration with the medical and biotechnology sectors.

[VII] The more applications/feedstocks there are (*), the more integrated the intermediate is; we counted three * for integration with "base chemicals"; see Appendix 2.

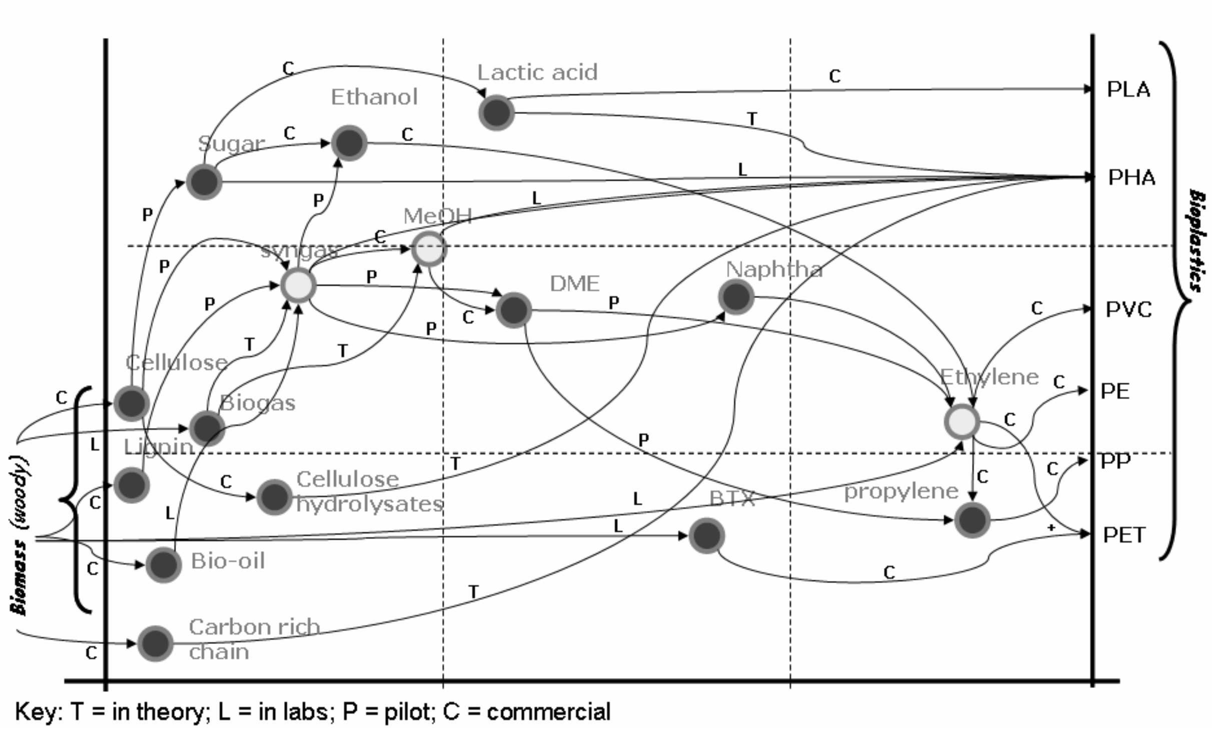


Figure 7: Intermediates with high integration levels are displayed as light dots.

The results of the last two steps of the analysis provide justification for including two kinds of routes in an environmental assessment: a) routes with high technology status/activity and low integration and b) routes with low/average technological maturity/activity but high integration. For example, the wood–sugar–ethanol–ethene–polyethylene route has a high technology status/activity level (i.e., ethanol dehydration plants are in operation in Brazil) and low integration (the various intermediates are poorly integrated with other sectors) compared to the wood–syngas–DME–ethene–polyethylene route, which has a low/average technology status (i.e., no existing industrial direct DME synthesis or MTO) but a highly integrated succession of intermediates (syngas, DME, and ethylene have numerous applications in various sectors). All these routes have good reasons for being environmentally assessed, which means that we will not fall into one of the traps outlined in section 2 because of using "unorganized" information.

Superimposing steps 1 to 5 allows us to gauge and identify the potential of different routes to bioplastics. Each of them has very good reasons for being environmentally assessed, for example, good technological maturity, high technological activity, and good integration with other industrial sectors. However, the "fashionability" factor of each intermediate has not been taken into account, and that is what we will deal with in the next step.

Step 6: Public expectations

As a final step, we gauge our intermediates with reference to public expectations as revealed in public statements, corporate strategy reviews, conferences, and media announcements. This is naturally the last information analyzed and gauged, since we have used a bottom–up strategy (see section 3). The importance of public expectations no longer needs to be demonstrated: it is a fact that some products have been ejected from the market because they were simply not fashionable enough, despite their superior technical properties.[9] This fashion factor could well have a great influence on the development of some routes to bioplastics.

Since we have by now looked at all the other indicators, we know that we have reduced the risk of making a mistake by unintentionally choosing an overly specific (too futuristic, not-for-profit based, etc.) scenario/technology in making an environmental assessment. The public expectations-gauging step is the final one, and gives an idea of the “trendiest” routes to bioplastics. Public expectations are measured by press releases, conferences, and other media announcements. Although there are more sophisticated ways to map expectations, a simple “googling” may be sufficient to illustrate this step.

Such an analysis aims to give an idea of what the “popular” intermediates are, so as to keep routes/intermediates that have attracted maximum public expectations. The intermediates favored by the public (see figure 8) are cellulose, ethanol, and syngas; thus, routes using those intermediates could be advantageous (see routes going through the light dots in figure 9). This supplies a final reason for environmentally assessing some routes within a pool of future biomass-to-plastics routes. These routes could be poorly supported by other factors (e.g., technology status and R&D activities), but if they are very fashionable, they should be included in the pool of environmentally assessed routes.

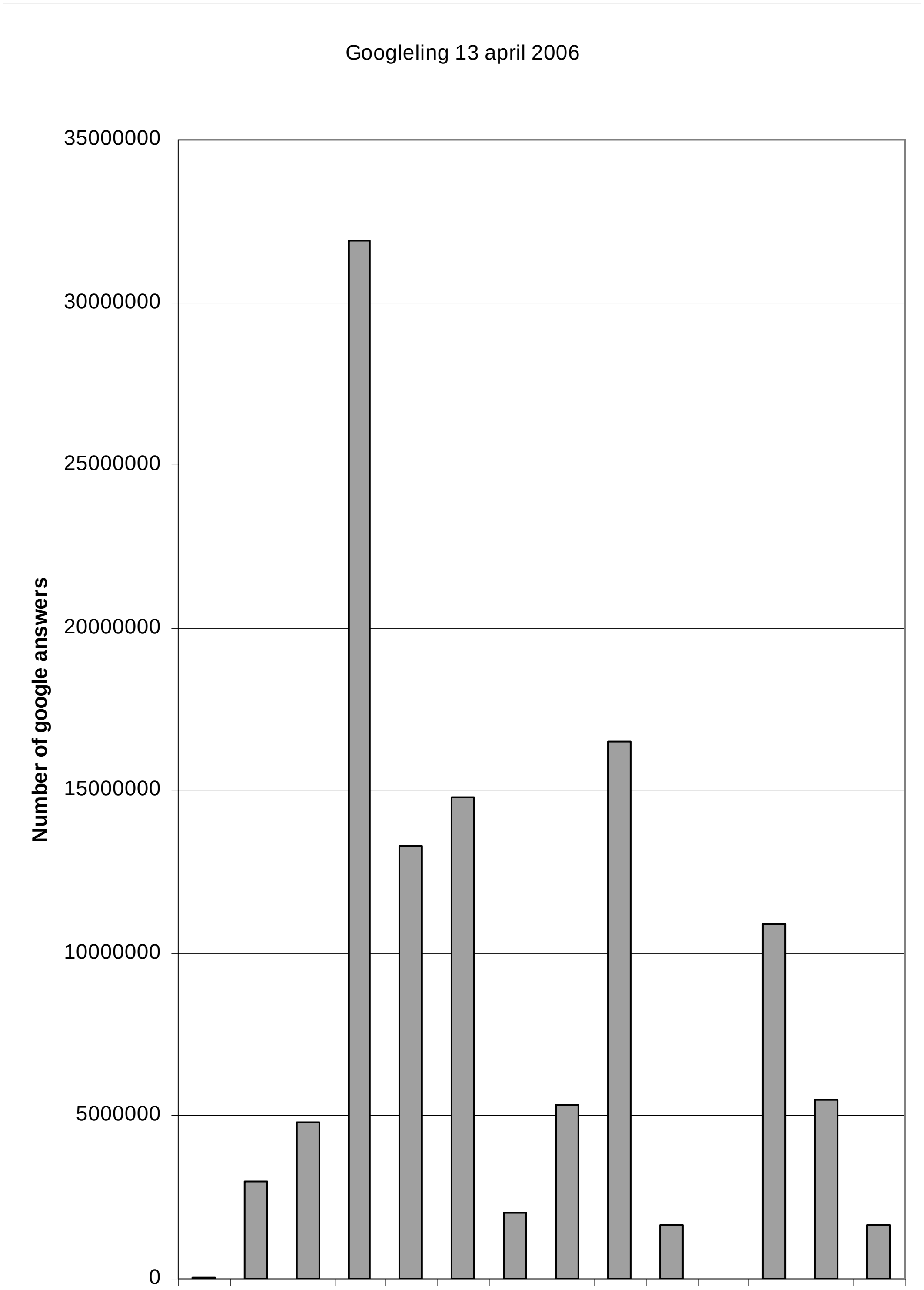
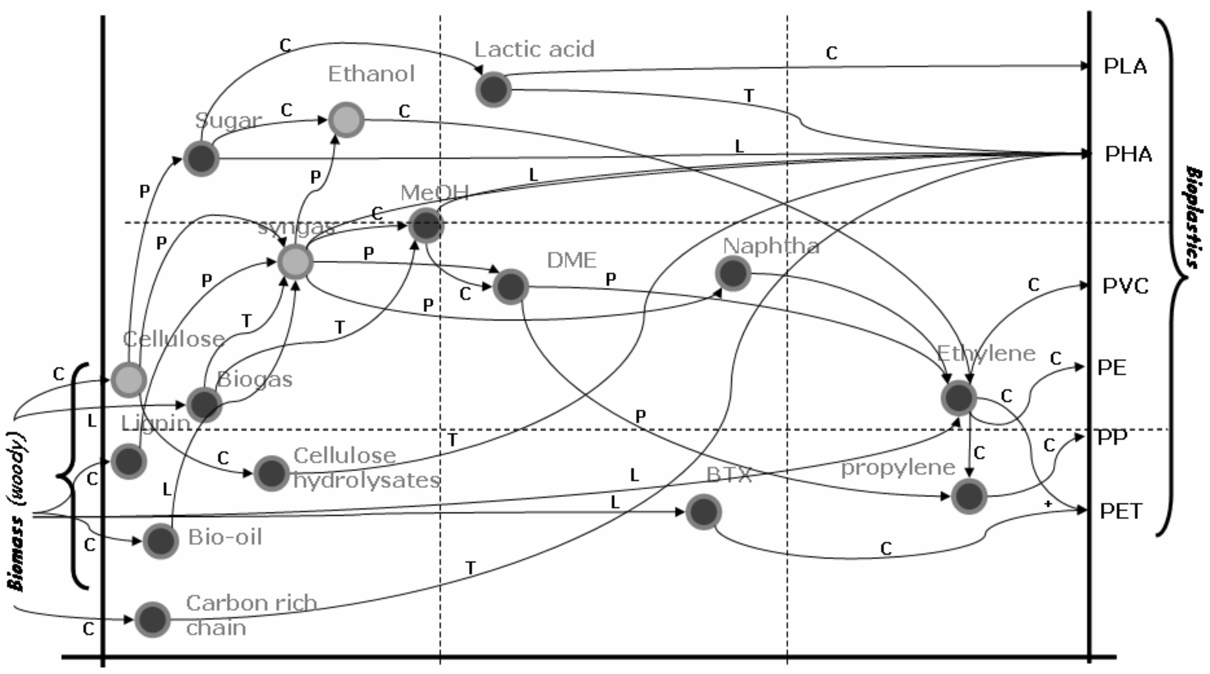

Googleling 13 april 2006
35000000
30000000
25000000
20000000
15000000
10000000
5000000
0
Number of google answers
Bio-oil
lignin
Bio-gas
Ethanol
Methanol
Cellulose
Sugar (hexose+pentose)
Lactic acid
Syngas
DME
BTX + aromatics
Ethylene
Propylene
Naphtha
Intermediates

Figure 8: Popularity of various intermediates determined using the Google search engine. The columns display the number of hits obtained when the name of the intermediate is entered in Google.



Key: T = in theory; L = in labs; P = pilot; C = commercial

Figure 9: Gauging each intermediate’s level of public expectations. The three most popular intermediates are indicated in light dots

Finally, the biomass-to-plastics mapping and gauging method gives us a number of coherent pathways extending from biomass to plastics using organized data that can be further used for environmental assessments. This method ensures the selection of a pool of routes via intermediates, which ultimately produces a meaningful comparison even though the technology statuses or production levels of the individual routes may differ. There are reasons why each of the routes should potentially be environmentally assessed, reasons that can be traced through the steps described above. One of the routes of interest for environmental assessment—highlighted using our method (see figure 10)—is that running from biomass, through syngas via gasification, then methanol and DME, followed by ethylene and propylene via MTO, and finally reaching plastic production.

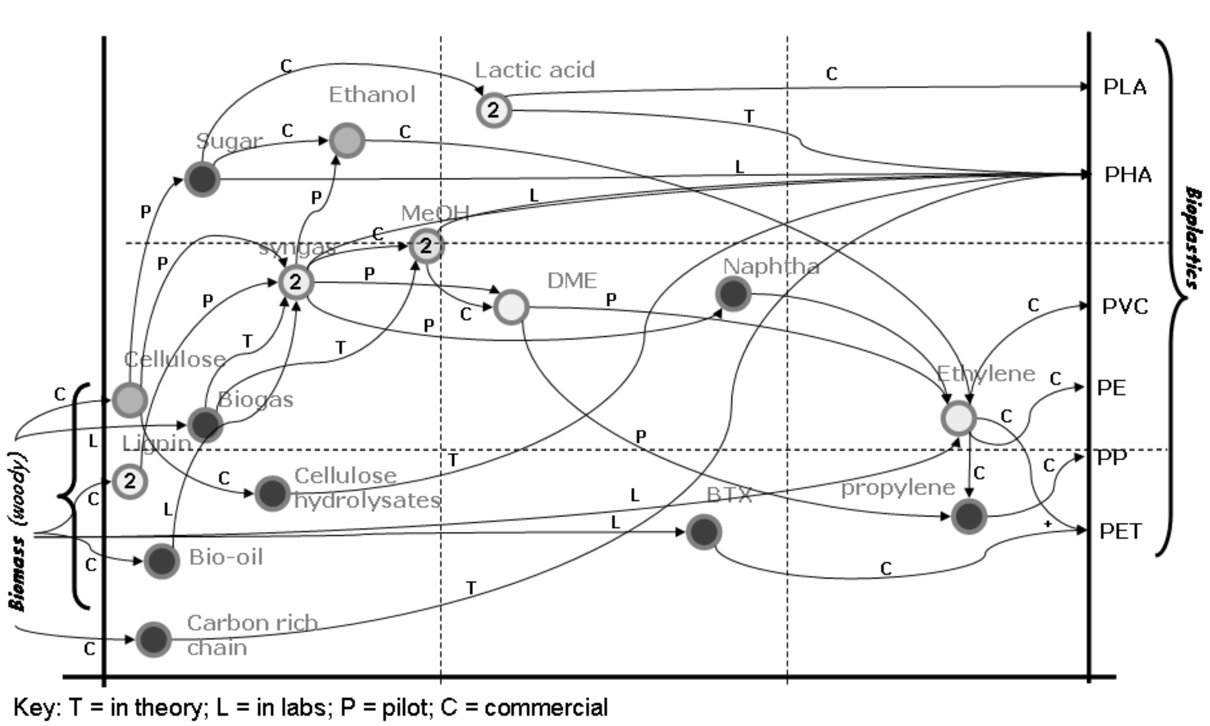


Figure 10: Superimposing all gauging indicators. The light dots show intermediates favored by an indicator. Numbers inside the dots show the number of indicators (starting at 2) favoring the intermediate.

4 With or without it

Using the presented method helps us avoid “missing” important information and prevents us from using “unorganized” information when using technology screening for environmental assessment purposes. Regarding missing information, using our method for bioplastics assessment would have prevented the European Commission IPTS team from missing the syngas-based processes that are omitted from their report.[4] In steps 3 and 5 of the method, the importance of syngas as an intermediate associated with bioplastic production has been made clear. Indeed, the syngas-based intermediates have such great potential—due to their cross-industrial integration (see table 3), for example—and are so popular in the alternative fuel sector (see figure 8), that it would be incoherent to omit them when assessing the environmental impacts and potential of bioplastic production.

As to the use of “unorganized” information, whether or not this method is applied will have a strong effect on the outcome of environmental assessments, suggesting that the wrong choice of method may lead to completely erroneous strategies. Here I compare the results of two LCAs, made without and then with the method, and highlight the differences between outcomes of the analyses. First, using technology screening data in the rough (as done by Edwards et al.[3]) for an LCA gives the following result for wood alcohol production: 87% of the total net nonrenewable greenhouse gas (GHGs) emissions come from collecting, chipping, and transporting biomass to the biomass-to-liquid (BTL) plant, while the rest comes from the gasification and fuel synthesis units (Edwards et al.[3]). This dominance analysis demonstrates that collection, chipping, and transport are the main sources of GHG emissions and therefore should be the first steps to be improved in dealing with total emissions.

However, using our method, the technology on which the above results are based is not selected. Indeed, in steps 1 and 2 of the method, the gasification configuration used in the study by Edwards et al is not kept as an option, since it does not stay within the chosen timeframe (standard b. in step 1). The gasification configuration used in the EUCAR study[3] is based on an excessively futuristic scenario in which electricity is produced on site using the feedstock, so it is not selected; other configurations associated with more coherent information are available. Using data pertaining to these routes (e.g., the Mitsubishi Heavy Industries Ltd. pilot in Chubu, Japan, or the Carbona Oy gasification configuration[10]) results in 90% of the net GHGs emissions coming from gasification and the rest from collection, chipping, and transport. This percentage results from the use of technology screening information with our method. Whereas the first results indicate that improvement should primarily be made in the logistics, the second ones would suggest focusing on improving gasification and the synthesis from syngas. Recent studies[11] have demonstrated that, indeed, logistics is of secondary importance in waste-to-products strategies. The method presented thus prevents our making strategic mistakes due to irrelevant results arising from the direct use of technology screening information in LCAs.

5 Conclusion

This paper aimed to develop a method for avoiding serious problems when conducting environmental assessment based on the screening of emerging technologies. These problems centered on factors such as anachronisms, omissions, and incoherencies. Using the proposed method, we can now justify the set of technologies assessed and answer questions concerning why specific products or processes merit study. The different steps of the method give different answers to such questions. Step 1 lets us answer, “because this product fits the specific feedstock, product, and time horizon definitions we established at the beginning of our study.” Step 2 lets us answer, “because it is a keystone to the routes we have identified.” Step 3 lets us answer, “because it has a commercial status.” Step 4 lets us answer, “because it has been the subject of much R&D.” Step 5 lets us answer, “because it is highly integrated with many other industrial sectors.” Finally, step 6 lets us answer, “because this product is very popular.” In the successive steps, information mapping has helped minimize possible omissions. Moreover, gauging the information gives real numbers justifying the selection of each of the products (or processes) for LCA study. As well as letting us answer such questions, thus strengthening the coherence of the environmental assessment, the method gives us a solid background for starting an environmental assessment of an emerging technology, such as bioplastics. Moreover, the method allows us to study derivations of the process (e.g., logistics and energy systems) and to change to different intermediates and reactions using the same line of reasoning: the derivations of the routes will still need valid reasons (e.g., technology status, popularity) for being chosen, within a defined and coherent background.

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Appendix 1: Market size and patents

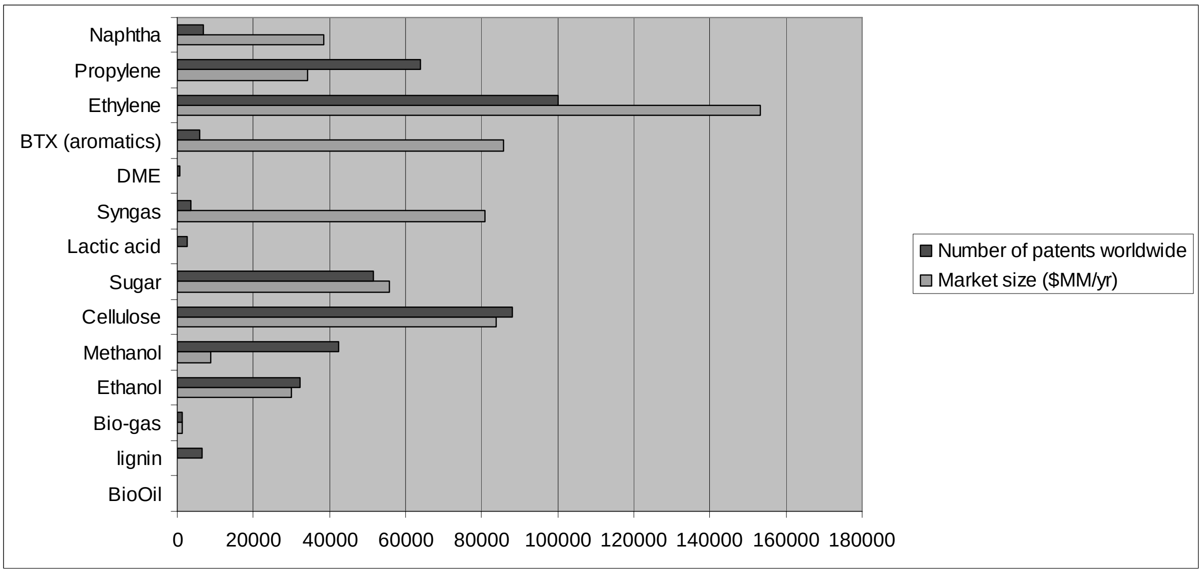

Figure 9: Market size and patent estimates for biomass-to-plastic intermediates

Appendix 2: Integration level of intermediates

Table 4: Intermediates with direct downstream applications (italics) and direct upstream precursors (the more applications and precursors there are, the more integrated the intermediate is).

Cellulose	**Lignin**	**Bio oil**	**CarbRich chain**	**Biogas**	**Sugar**	**Syngas**	**Cellulose hydrol.**	**Et OH**	**MeOH**	**Lactic acid**	**DME**	**BTX**	**Naphtha**	**C3=**	**C2=**
Biomass	Biomass	Biomass	Biomass	Biomass	Biomass	Biomass	Cellulose	Ethane	syngas	Sugar	Methanol	Oil	oil	DME	Biomass
Paper	*Dispersant*	*Fuel*	*Food*	*Fuel*	*food*	Coal	*fuel*	Biomass	*Acetic acid*	*PLA*	Syngas	coal	*Olefins*	Naphta	DME
textiles	*Emulsifier*	*Food products*		*Substrat*	*Substrat*	Nat. gas		syngas	*Formaldehyde*	*Food*	*Diesel*	*PET*	*Aromatics*	Propane	Naphta
	Fuel	*Resins*		*syngas*		waste		*Solvent*	*MTBE*	*Propylene glycol*	*Synthetic LPG*	*Styrene*		Butane	Ethane
	Sequestrant	*Polymers*				*Fuel*		*Ethylene*	*Fuel cells*	*Acrylic acid*	*Fuel cell*			Fuel oil	Propane
	Binder					*Base chemicals*		*Drink*	*Olefins*	*Polyesters*	*Olefins*			Ethylene +butylene	Fuel oil
								Fuel	*DME*	*Lactate esters solvents*				*PP*	*PE*
									Fuel						*Base chemicals*
															ethanol

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