Medium and Long-term Opportunities and Risks of the Biotechnological Production of Bulk Chemicals from Renewable Resources

- The Potential of White Biotechnology

The BREW Project

Final report

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Executive summary

In the last few years, enormous progress has been made in biotechnology including genetic engineering. Further major scientific and technological breakthroughs are expected for the coming years and decades. While biotechnology has already taken shape in the production of pharmaceuticals, fine chemicals and speciality chemicals and is expected to expand considerably in these sectors in the short to medium term, there is substantial uncertainty about when, how and to which extent biotechnology will also play a role in the production of *bulk* chemicals. High expectations are connected to the developments in this field of "White Biotechnology" with regard to their benefits for science, technology and society in the medium to long term. In the recent past important steps have been made in research, companies and policy, with the goal of developing White Biotechnology for the production of chemicals. While there is a strong drive behind these developments there is so far only very little quantitative information available in the public domain on the current and future economic, environmental and societal implications. This report is a contribution to close this gap of knowledge.

In terms of scope, this report studies processes which convert biomass-derived feedstocks (e.g. fermentable sugar) into *organic bulk* chemicals (e.g., lactic acid, acetic acid, butanol and ethanol) by means of White Biotechnology, i.e. by fermentation or enzymatic conversion, either *with* or *without* genetically modified organisms. Apart from White Biotechnology, also conventional chemistry is involved in all processes. All White Biotechnology products are compared to functionally equivalent petrochemical products. The focus is on industrial chemicals while food, animal feed and fuels *only* are excluded.

The key research questions addressed in this report are which products could be made with White Biotechnology, whether these products can contribute to savings of energy use and greenhouse gas (GHG) emissions, under which conditions the products become economically viable, which risks may originate from a shift towards White Biotechnology chemicals including the use of genetically modified organisms (GMO) in fermentation and what the public perception is.

In **Chapter 2** of this report, an overview is provided of chemicals which can be produced by White Biotechnology. Starting from an extensive list of possible bio-based chemicals (see Figure 2-1 and Table 2-28 and 2-29) a selection was made based on the product-tree approach, leading to a selection of 19 building blocks plus derivatives of natural fats and oils and finally genetically modified crop plants. These products have been discussed in detail in Chapter 2.1 to 2.7. For each product, the key features of production and use are discussed (e.g., biotechnological options, level of maturity, commercial status, world-wide production volume, challenges and drivers). Further assessment within the BREW team led to a selection of 21 products as top candidates for White Biotechnology (see Table 2-42; these products are analysed in-depth in Chapter 3 and 4). Two key strategies for their market entry are firstly *Direct substitution of a bulk petrochemical* and secondly *Functional competition of bio-based bulk chemicals with fossil-based ones*. Some of the selected 21 White Biotechnology chemicals belong to both categories.

Based on the insight gained in Chapter 2 we conclude that **White Biotechnology offers numerous opportunities for the manufacture of new and existing organic bulk**

chemicals from a variety of feedstocks and that, given the early stage of development for most products and processes, **very substantial progress can be expected** for the future. **According to our assessment, the large-scale manufacture of White Biotechnology chemicals is technologically challenging but there is a wide range of interesting options and it does seem feasible for the longer term.**

While, from a (bio-)chemical and a technological point of view, the opportunities are interesting and promising, the attractiveness for industry and policy depends to a very large extent on whether White Biotechnology products offer advantages in economic and in environmental terms.

In **Chapter 3** we therefore conduct detailed environmental and economic assessments (in specific terms, i.e. per tonne of product) for the 21 White Biotechnology products selected in Chapter 2. So far, quantitative analyses on the environmental impacts and the economic aspects related to bio-based bulk chemicals produced by White Biotechnology are scarce, fragmented and incomparable due to different assumptions and boundary conditions. In contrast, we apply a uniform methodology with common background data (BREWtool). We conduct our analyses for different prices for fermentable sugar but only one oil price (US$ 25/barrel crude oil; for natural gas, a price of 4 €/GJ was assumed for final users in the chemical sector; Appendix A3-2). Chapter 3 discusses also the so-called Generic Approach which is the methodology we developed and applied to assess future processes, for which very little information is available.

In summary, our finding is that White Biotechnology for bulk chemicals production is **primarily an economic challenge** while it **offers very substantial opportunities for the chemical industry to reduce their non-renewable energy use, greenhouse gas emissions** and related environmental impacts. Nearly all of the products studied are environmentally attractive (non-renewable energy use and greenhouse gas emissions) already with *current* technology and using maize as feedstock (30% cradle-to-factory gate non-renewable energy savings as arithmetic mean without adipic acid and acetic acid compared to petrochemicals), and even more so in future (50% energy savings). Larger savings are achieved if lignocellulosic feedstocks can be used in future (up to 75% non-renewable energy savings) and even higher savings can be realized if fermentable sugar from sugar cane is used, where for future technology up to 85% non-renewable energy can be saved on average compared to the production of petrochemicals nowadays. Moreover, White Biotechnology chemicals score clearly better than liquid biofuels (ethanol) with regard to the non-renewable energy savings per unit of agricultural land used (GJ energy saved per hectare land used).

The *economic* challenge of White Biotechnology chemicals in competition with their petrochemical counterparts is closely linked to technological progress. In conclusion, technological breakthroughs (both in the bioprocess step and in product separation and purification) are more important in order to achieve economic attractiveness than to improve environmental attractiveness.

In **Chapter 4**, three scenario projections are developed for Europe (EU-25) until the year 2050. We distinguish between a scenario LOW with rather unfavourable conditions for bio-based chemicals (oil price up to 30 US$/barrel; sugar price of up to 400 €/t; 0% p.a. physical growth in the chemical sector), a scenario MEDIUM (up to 66 US$/barrel,

up to 200 € /t sugar and 1.5% p.a. physical growth of organic chemicals) and a scenario HIGH (up to 83 US$/barrel, approx. 70 €/t sugar and 3.0% p.a. physical growth of chemicals).

Absolute non-renewable energy savings for Europe (EU-25) depend on the scenario chosen. In the scenario LOW in 2050, about **7%-10%** of the non-renewable energy demand for the (conventional) production of the selected chemicals studied are saved, while in the scenarios MEDIUM and HIGH this percentage is about **20%-30%** and **39%-67%**, respectively (lower values for starch, higher values for lignocellulosics; see Section 4.5.2 and Appendix 11-13). In other words, up to two thirds (67%) of the current non-renewable energy use for the production of the selected chemicals could be saved by 2050 if substantial progress is made in White Biotechnology and if the use of lignocellulosic feedstocks is successfully developed. Instead of comparing the savings of energy and GHG emissions to the *production of the selected chemicals*, they can also be compared to the *total production of all organic chemicals*. In this case the saving percentages are roughly half of the ones just quoted.

The total land use for bio-based chemical production is relatively low in most scenarios. If starch is used as basis for fermentable sugar, the total land use ranges from 1.0 to 38.1 million ha in the three scenarios. If lignocellulose is used as biofeedstock, only 0.4 to 15.6 million ha are needed. For comparison, the agricultural area in the EU-25 was about 180 million ha in 2002. Land requirements are hence not likely to become a critical issue in the next few decades (Section 4.5.2).

In 2050, White Biotechnology hence offers substantial macroeconomic savings in the scenarios MEDIUM and HIGH (6.7 and 74.8 billion €) while it entails relatively small additional expenses in the scenario LOW (–0.13 billion €, see Section 4.5.2). The macroeconomic savings imply improved international competitiveness. The annual added value of the bio-based chemicals is estimated for 2050 at about 1.8, 8.8 and 33.2 billion € in the scenario LOW, MEDIUM and HIGH respectively.

We conclude from Chapter 4 that, under favourable conditions (see also the four requirements given at the end of this executive summary), White Biotechnology becomes a reality, enabling substantial savings of non-renewable energy use and greenhouse gas emissions, parallel to economic advantages. Given the scenario results we conclude that the large-scale production of White Biotechnology products will most likely occur first in countries with low prices for fermentable sugar (in particular, in Latin America). European industry is likely to develop White Biotechnology in Europe, to apply it first on a large scale abroad and finally to exploit its opportunities in Europe.

In **Chapter 5**, the risks related to the use of White Biotechnology are studied. The main purpose of this chapter is to give insight into the main risk components influencing the overall risk and of the knowledge gaps. Both conventional risks (e.g., human toxicity and accidents) and risks related to generic modification (e.g., horizontal gene transfer) are analyzed:

- **Conventional risks** of biotechnologically produced chemicals (risks related to genetically modified micro-organisms and crops excluded) are found to be comparable to those of chemicals derived from fossil fuels); however, if White Biotechnology materializes, new raw materials, intermediates and final products

will be handled and as a consequence, suitable safety procedures need to be developed.

- The **risks related to the use of genetically modified organisms** in White Biotechnology are manageable if adequate precautionary measures are taken; in view of existing knowledge gaps, the specification of these measures requires further work; the challenges are larger for Green Biotechnology compared to White Biotechnology, which is hence closer to large-scale production in chemical industry.

In **Chapter 6**, public perception and stakeholder perception is discussed because this may play an important role for the implementability of White Biotechnology on a large scale. We conclude that stakeholders and the public seem to have a **basically positive attitude** towards organic chemicals made from White Biotechnology, with environmental considerations and the use of renewable raw materials primarily determining this perception. This conclusion is, however, based firstly on studies which partly have a different scope than the BREW study and secondly on the BREW survey among stakeholders which may differ from the perception of the public. While more certainty can hence only be ensured by means of a study dedicated to public perception, the available information indicates that public perception is no critical issue and is, on the contrary, supportive under current circumstances.

Finally, the findings are summarized and conclusions are drawn in **Chapter 7**. It should be kept in mind that the **assumptions made in the BREW study** for the future with regard to the bioprocess (see especially Table 3-2) and downstream processing are crucial for the outcome of the calculations. Moreover, **innovations in fossil-based chemicals production** have not been taken into account in the BREW project, including the production of olefins from coal, which could become the largest menace to (bio-based) White Biotechnology for bulk chemicals.

We conclude from our analysis that the following **four core requirements** must be fulfilled in order to make clear steps towards a bio-based chemical industry, namely:

1. **Substantial technological breakthroughs in the bioprocess step**
2. **Major progress in downstream processing**
3. **Prices for fossil fuels must be high.**
4. **Prices for fermentable sugar must be low.**

For each of these factors we provide suggestions for measures which could be taken and we propose **accompanying activities** (see Chapter 7.2).

To conclude, we strongly recommend to **develop an integrated White Biotechnology strategy** taking into account the four core requirements and the proposed accompanying activities, provided that the European Union arrives at the conclusion to actively support White Biotechnology.

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1. Introduction

In the last few years, enormous progress has been made in biotechnology including genetic engineering. Further major scientific and technological breakthroughs are expected for the coming years and decades. To date, industry has focused most of its attention regarding biotechnology on two areas, i.e., the production of food and animal feed on the one hand and medical applications on the other. The public discussions concerning genetic engineering have also been dealt with issues in these two domains, with human genomics playing a more and more important role in the recent past. Apart from food and animal feed production and medical applications, biotechnology is about to open new perspectives also for the manufacture of chemical bulk materials and intermediates. High expectations are connected to these developments with regard to their benefits for science, technology and society in the medium to long term (EuropaBio and ESAB, not dated; EuropaBio/ESAB/SusChem 2005, not dated Eur. Commiss. 2002; Eur. Commiss. 2004; OECD 2001; BACAS 2004; Dechema 2004; Ast et al. 2004; Gavrilescu and Chisti 2005; Willke and Vorlop 2004; Wagner et al. 2004; Hoppenheidt et al. 2004; Werpy and Petersen 2004).

Plants, which use the sun's energy to convert CO_2 into polysaccharides and other complex molecules, have tremendous potential to be used as sustainable raw materials for the biotechnological production of chemical bulk materials and intermediates. This is especially true if plant products are adapted more precisely to the needs of the respective biotechnological processes. Biotechnology is expected to play a key role for the cleaner production of bulk chemicals, with important reasons being the use of a renewable resource base as a feedstock and the reduction of emissions (including CO_2) and noxious waste throughout the life cycle (e.g., OECD 2001). Biotechnology can be used to produce various bulk chemicals that are currently produced from fossil feedstocks and, possibly more efficiently, for new building blocks ("platform chemicals") that can serve as starting materials for many other materials provided that they are cost competitive.

Already today, some chemical companies have made major investments into R&D and industrial production in order to exploit biotechnology for the production of chemicals (Degussa, DSM, DuPont, NatureWorks, Novozymes). Interestingly, high potentials of biotechnology for chemical industry are expressed by actors with otherwise strongly differing agendas, e.g. the European chemical industry federation (CEFIC 2004) and some environmental political parties (e.g., the Green party in Germany, Bündnis 90/Die Grünen). The European Commission has put the biotechnological production of bulk chemicals on their research agenda not only for the present 6th Framework Programme but also for the coming 7th Framework Programme (compare EuropaBio, 2005). Moreover, sizable R&D activities have been launched in some European countries (e.g., an integrated institute for industrial biotechnology is being set up in the Netherlands; Task Force Ind. Biotechnology, 2005).

This indicates that there is a strong drive behind the development of biotechnology for chemical industry and also a broadly supported positive attitude towards these

opportunities. Amazingly, there is, however, only very little quantitative information available in the public domain on the current or future expected economic and environmental advantages. Studies that do provide quantitative information are often based on a very small number of case studies for which, not rarely, the basic assumptions are not specified (e.g., OECD 2001). Private consultancies have prepared reports on the state –of –the art and the prospects of biotechnology (e.g., SRI-PEP 227 1999; SRI-PEP 236 2001; SRI-PEP 188B 2002), which contribute substantially to a better understanding of the present situation and the future development potential of the use of biotechnology for industrial products. However, most of these reports are available only at high cost, which limits their dissemination and is hence also prohibitive to an open discussion and the development of joint strategies between companies and governments.

This shows that there is a clear information gap, which is in contrast to the need for well-founded decisions on the public and the private side. Early discussions in the public sphere and surveys among representative sample groups can help to avoid incomplete understanding and false expectations regarding the public perception. For these purposes, publicly available information on the topic must be at hand.

Next to processing renewable raw materials by means of *biotechnology*, other (non-biotechnological) process routes to produce bio-based chemicals are

- the direct use of compounds found in nature and their modification (e.g., of starch to produce thermoplastic starch) or
- thermochemical conversion processes (e.g., fast pyrolysis of biomass to produce aromatics or biomass gasification with subsequent C_1 chemistry).

While there are very interesting and successful first examples in these two areas (compare e.g., Bastioli 2005 and Crank et al. 2005; Hamelinck and Faaij 2002) this report deals with the application of biotechnology for the production of organic bulk chemicals.

Within biotechnology, the distinction is made between Green Biotechnology, Red Biotechnology and White Biotechnology. Green Biotechnology deals with the use of genetically modified crops (nowadays mostly for food and animal feed), Red Biotechnology deals with medical applications and White Biotechnology with the application of fermentation and enzymatic processes for industrial products and fuels. White Biotechnology may or may not make use of genetically modified organisms.

This report deals with White Biotechnology, which is referred to as Industrial Biotechnology in the U.S.A. While Green Biotechnology can also be applied to produce chemicals (e.g., polyhydroxyalkanoates which are polyesters) or feedstocks for thermochemical or fermentation processes, these options are beyond the scope of this study. Nevertheless Green Biotechnology is discussed in some parts of this report for comparative purposes (especially in the context of risks and public perception in Chapter 5 and 6). White Biotechnology has been chosen as the subject matter of this study because, for the medium term, chemical industry generally considers this route to

be technologically more viable than Green Biotechnology and because public opposition to the latter is expected to be substantial.

1.1 Objective and scope of the project

This study investigates the medium and long-term opportunities and risks of the biotechnological production of organic chemicals. The **objective** is to gain better understanding of the techno-economic and the societal viability of White Biotechnology in the coming decades. The key research questions are which products could be made with White Biotechnology, whether these products can contribute to savings of energy use and greenhouse gas (GHG) emissions, under which conditions the products become economically viable, which risks may originate from the use of genetically modified organisms (GMO) in fermentation and what the public perception is. The **scope** of the analyses conducted to answer these questions are:

- In terms of technology, all options studied should contain at least *one* process step that involves White Biotechnology, i.e. either fermentation or an enzymatic conversion either *with* or *without* genetically modified organisms. In addition, one or more conventional chemical conversion processes may be involved.
- While both fossil and bio-based feedstocks can be processed with White Biotechnology, the BREW project studies only bio-based products made from renewable resources (bio-based feedstocks) because these offer larger potentials for energy saving and GHG abatement. All White Biotechnology products are compared to functionally equivalent petrochemical products.
- While some first large-scale processes applying White Biotechnology already exist, this technology is still in an infant stage. Both the current state –of –the art and the future situation are assessed in this study. For the future, assumptions are made for the expected state of White Biotechnology and for the enabling downstream processing technology in two to three decades from now (around 2020-2030). Implementation of this technology will require additional time. Therefore, the entire timeframe covered in this study reaches up to the year 2050.
- In order to assess whether meaningful energy savings and GHG emission reductions can be achieved, this study analyses *bulk* products made by White Biotechnology. Bulk products are defined here as having a production volume in Western Europe of 20-50 kt per year by 2020 (1 kt = 1 kilotonne = 1,000 metric tonnes) but ideally, being of much larger size, in the range of at least 200 kt. Niche products with high prices are not included.[1]

[1] The smaller scale of 20-50 kt p.a. is applied in Chapter 2, the purpose of which is to give an overview of (potentially) emerging bio-based products while the model and scenario analyses presented in Chapter 3 and 4 deal with products which are expected to be produced at least at a scale of 200 kt p.a.

- Only products should be included which belong to the core business of the chemical industry. Therefore products such as food, animal feed, paper and textiles are not included. Also products which are used as fuels *only* are excluded. In contrast, products such as ethanol that are used both as chemicals and as fuels are included.

To summarize, the products studied in this report are bulk bio-based organic chemicals produced by means of White Biotechnology. For simplicity, we refer to these products as *bio-based products, bio-based chemicals* or *White Biotechnology products* (these terms are used as synonyms). These products are compared to equivalent petrochemical products.

Bio-based chemicals are receiving increased attention in industry and in government policy. We therefore discuss bio-based chemicals from these two perspectives in the next two sections (Section 1.2 and 1.3).

1.2 Why bio-based? – The company perspective

By far the largest amounts of organic chemicals are nowadays produced from petrochemicals and clearly, the most important reason for companies not to shift to bio-based production on a large scale is the higher production cost. Only in *exceptional cases* bio-based products are at a similar level as or even outpace chemically identical products made from petrochemical feedstocks, with ethanol being the key example: Worldwide, at least ten times as much ethanol is nowadays produced biotechnologically from bio-based feedstocks (mainly based on maize starch and sugar cane) than from petrochemical ethylene made in steam crackers.[2] A more recent example is 1,3-propanediol (PDO): Shell produces PDO from petrochemical ethylene oxide (SRI-PEP 227 1999) whereas DuPont is currently building a plant for PDO production from maize-based glucose (Muska and Alles 2005). Different economic evaluations have led here to different feedstock choices. Competition on a *functional* basis without chemical identity is more frequent (e.g., for surfactants based on vegetable oil and for polylactic acid versus polyethylene terephthalate). In some cases the bio-based products have additional functionalities, leading to higher value products (e.g., chiral products or biodegradable plastic packaging). In niche markets, the use of bio-based feedstocks *as such* allows producers to fetch a higher price for their product due to the green image which these products carry.

Higher profit margins due to lower production cost, additional functionality or green image might become increasingly important in the bulk organic chemical business where the high performance of the conventional products (e.g., standard polymers), in combination with the fierce competition (leading to low prices and dwindling profit margins) makes it more and more difficult to develop and launch totally new products.

[2] According to Weissermel and Arpe (2003), world-wide 24.1 million tonnes of bioethanol were produced in 1997, while the global production of petrochemical ethanol made from ethylene in steam crackers amounted to 2.6 million tonnes in 1998. According to Berg (2004) the world-wide production of ethanol in 2003 totalled approximately 31.5 million tonnes (Berg 2004).

For example, practically all bulk polymers, that are nowadays used, have been developed 45 to 80 years ago and it is questionable whether any new bulk plastic will be commercialized in the future (Lemstra 2005). Bio-based chemicals might hence help to renew the chemical sector. At the same time, the tight business conditions make it even more difficult for bio-based chemicals to compete.

It seems that this ambivalent overall situation has led to rather diverse business strategies in the chemical sector. For example, DSM and Degussa have been moving away from the petrochemical business in order to focus on fine chemicals, in particular produced with White Biotechnology. NatureWorks LLC[3] is the first company producing a bio-based polyester (namely polylactic acid, PLA) in a world-scale industrial plant (140 kt p.a. capacity). This has boosted the interest in bio-based polymers in general and in PLA in particular and may well have been a key driver for other companies, research institutes and public funders to seriously consider or even to invest in bio-based chemicals. NatureWorks sees polyethylene terephthalate (PET) as an important target market for their products and competition on cost basis is already reality today. PLA products are making inroads in markets where retailers and brand owners recognize the value of more sustainable polymers and the use of renewable raw materials. But PLA products have to compete with existing polymers and the rapid expansion of the PLA market remains a challenge.

Next to companies like Degussa, DSM and NatureWorks which have invested heavily into bio-based chemicals, an increasing number of large companies seems to be exploring the field and making first cautious steps.[4] On the other hand, many big players in the chemical industry do not seem to see much opportunities for large-scale bio-based chemicals, at least not in the short to medium term. The diverse expectations among companies calls for further analysis.

1.3 Why bio-based? – The policy perspective

The key policy goals to which bio-based materials can, in principle, contribute are energy savings (fossil energy), greenhouse gas (GHG) emission reduction, supply security, innovation and moreover, growth and employment in the chemical sector and in agriculture. Life cycle assessment studies (LCA) for bio-based polymers show that attractive energy savings and emission reductions can be achieved in *specific* terms - i.e., per kg of product (Patel et al. 2003). Since, however, the market quantities of bio-based polymers that are commercialized today or that are close to commercialization are not expected to exceed 2-3 million tonnes in Europe 15 until 2020 – representing 4.4%-

[3] Until early 2005 named Cargill Dow (a joint venture of Dow Chemical and Cargill)

[4] On the other hand, BP recently entered a collaboration with Metabolix for the switchgrass-based route to PHA (Green Biotechnology; Tullo 2005); BASF announced that it will launch a biodegradable plastic based on renewable raw materials (BASF 2005); and Archer Daniels Midland (ADM) and Metabolix will set up a plant for polyhydroxyalkanoates (PHA) with a production capacity of 50,000 tonnes per year (ADM 2006; Metabolix 2006).

6.7% of the current polymer market (approx. 45 million tonnes in Western Europe in 2000) – the savings in absolute terms are rather small. Until 2020, they are expected to represent not more than 5% of the current CO_2 emissions of the chemical sector (year 2000); and compared to the current CO_2 emissions of the *total economy*, the projected savings due to bio-based polymers are not more than 0.2% (Crank et al. 2005). These shares refer to commercialized and nearly commercialized bio-based *polymers* only. The extension to *all* organic chemicals (including polymers) that are on the market or close to commercialization is expected to lead to very similar conclusions because polymers represent the most important group of organic chemicals. While it may be argued that the savings are hence too small to consider bio-based chemicals as a meaningful strategy for abating greenhouse gas emissions, this seems to be a too quick conclusion given the early stage of development of bio-based chemicals and the challenge of realizing substantial changes in the (existing) chemical industry. More time is required for developing and implementing advanced technology. Given that climate policy is likely to be a task for many decades to come in *all* sectors of the economy and given also that technological progress could be accompanied by many further benefits (e.g., economic growth and employment), it may well be worthwhile to launch ambitious programmes in the next few years. In particular White Biotechnology is generally seen as very promising option in terms of environmental, economic and social benefits. Already the final report of the European Climate Change Programme, which ran from mid-2000 to mid-2001 and was set up to identify the most cost-effective and environmentally beneficial measures enabling the EU to meet its greenhouse gas emission reduction target, pointed to the biotechnology for the production of bulk chemicals from biomass feedstocks (ECCP 2001). Moreover, there are important synergies with renewable energy, because bioethanol for fuel purposes is produced biotechnologically and rapid expansion is expected in Europe as consequence of ambitious European policy making (Eur. Commis.-ETAP Newsletter 2005; Official Journal of the EU 2003). For biodiesel, which is produced by means of conventional catalysis from rapeseed oil in several European countries, White Biotechnology (here: enzymatic conversion processes) could improve the relative position.

Apart from environmental advantages (waste minimization, lower energy use, substantial GHG emission reduction by 2010) White Biotechnology is, according to EuropaBio (2003), key to the competitiveness of many of Europe's industries, i.e., chemicals, textiles and leather, animal feed, pulp and paper, energy, metals and minerals, as well as waste processing. According to McKinsey & Company 2003 (quoted in EuropaBio 2003) White Biotechnology could be applied for the production of 10 to 20% of all chemicals sold by the year 2010 and it could generate an additional added value of up to 11 to 22 billion € per annum by 2010. Roughly half of this increase in value added is expected to be enabled partly by lower costs for raw materials and processing while the other half is generated by additional revenues from new products or products with enhanced performance (McKinsey & Company 2003, quoted in EuropaBio 2003).

Policy at the European level and in its member states strives to ensure optimal conditions for their industries in order to foster competitiveness and growth, while

simultaneously pursuing environmental goals. It is therefore of interest to understand which role current and possible future boundary conditions have and how policy would need to change these. One of the most important changes for Europe in the next decades is the integration of the Eastern European countries which could play an important role in supplying and processing large amounts of bio-based feedstocks at low cost. Among the policies and measures which may have the strongest influence on the economic viability of White Biotechnology products are measures to ensure access in the European Union to agricultural products at world market prices or the modification of the product refund. In addition, governments may extend their R&D for White Biotechnology (and possibly other bio-based chemicals) if the prospects continue to be promising and if additionality can be ensured. When deciding about whether or not to support White Biotechnology and bio-based chemicals governments will, moreover, have to take into account the public perception of these products.

1.4 Structure of the report

Apart from the introductory chapter (Chapter 1) this report is divided into six chapters. The main purpose of **Chapter 2** is to provide an overview of emerging key White Biotechnology products and to explain which chemicals could be produced on their basis. For a selection of these products, detailed environmental and economic assessments are conducted in **Chapter 3** (in specific terms, i.e. per tonne of product). Chapter 3 discusses also the so-called Generic Approach which is the methodology we developed and applied to assess future processes and processes, for which very little information is available. In **Chapter 4**, three scenario projections are developed for Europe (EU-25), thereby assuming benign, moderate and disadvantageous conditions for bio-based chemicals. The purpose of this chapter is hence to understand to which extent restructuring of the chemical sector might occur under which conditions. In **Chapter 5**, the risks related to the use of White Biotechnology are addressed. The main purpose of this chapter is to give insight into the main risk components influencing the overall risk and of the knowledge gaps. Both conventional risks (e.g., human toxicity and accidents) and risks related to generic modification (e.g., horizontal gene transfer) are analyzed. Since the public perception may play an important role for the implementability of White Biotechnology on a large scale, these issues are discussed in **Chapter 6**, thereby drawing conclusions from the literature and presenting the outcome of a survey. Finally, the findings are summarized and conclusions are drawn in **Chapter 7**.

2. Emerging White Biotechnology products[5]

This chapter provides an overview of biotechnological processes for bulk chemicals and intermediates (see scope definition in Section 1.1). The goals of this chapter are to

- provide a comprehensive overview of relevant processes and products and to outline the technological potential of biotechnology in this field,
- to compile information which is now scattered over different sources,
- to give a structure and organise the processes/products into appropriate categories,
- to provide a basis for putting selected cases and results from the following chapters into perspective.

This chapter is organised by types of building blocks. We define building blocks as chemicals derived from biomass by application of biotechnology. Building blocks usually form the basis of interesting product trees when further processing (conventional chemical or biotechnical processing) is applied (Linton, Nisbet 2000). They therefore have the potential to be produced on bulk scale, at least in the longer term future. While the exclusive use of compounds as fuels, animal feed or food ingredients falls outside the scope of the definition of a building block, important uses are mentioned in this Chapter 2 in order to provide a more complete picture.

In order to identify chemicals falling into the scope of this study (Section 1.1) we performed a screening process consisting of the following elements:

- Identification of biotechnologically produced chemicals, which are produced from biomass on a bulk scale already today,
- Identification of bulk chemicals which are produced chemically from fossil resources today, but which could possibly also be produced from biomass with biotechnological steps,
- Identification of bio-based, biotechnologically processed (novel) products which are functionally equivalent to existing, fossil-based products,
- Identification of bio-based, biotechnologically processed building blocks which could give rise to various chemicals and may therefore be needed in bulk quantities.

Figure 2-1 presents the outcome of this screening process. Starting from the main constituents of biomass, namely from the carbohydrates sucrose, starch, cellulose and hemicellulose, from lignin, oils and protein, biotechnological processes are shown that are or could be established for the conversion of these main biomass constituents. No attempt was made to achieve completeness for substances that are fine or speciality chemicals or are mainly used for food purposes because these substances are beyond the scope of the BREW project. The substances listed in Figure 2-1 were then

[5] The author of this chapter is Dr. Bärbel Hüsing, Fraunhofer Institute for Systems and Innovation Research, Karlsruhe, Germany.[6] Based on the theoretical maximum yield of 511 g ethanol/kg glucose (following Wheals et al. 1999).

complemented by chemical compounds that can be obtained via chemical and/or biotechnical conversion.

In another analytical step, these substances were sorted into product trees from which building blocks were chosen for further analysis by applying the following criteria:

- Potential of the building block or its derivatives for direct or functional replacement of petrochemically derived bulk chemicals,
- Potential of the building block to provide the basis of a diverse product portfolio, e.g. due to chemical functionality and potential use,
- Strategic fit with market perspectives and main drivers of future development,
- Technical complexity of synthetic routes from biomass to building block and from building block to derivatives.

On this basis, building blocks were selected for further analysis. They are described in the following sections, which are ordered by increasing number of carbon atoms in the compound.

The approach and criteria chosen in the BREW project are similar but not identical to those employed in the recent report by Werpy and Petersen 2004. Werpy and Petersen aim at identifying top value added chemicals from biomass. Their analysis therefore leads to a somewhat different list of promising building blocks compared to our analysis which focusses on bulk applications.

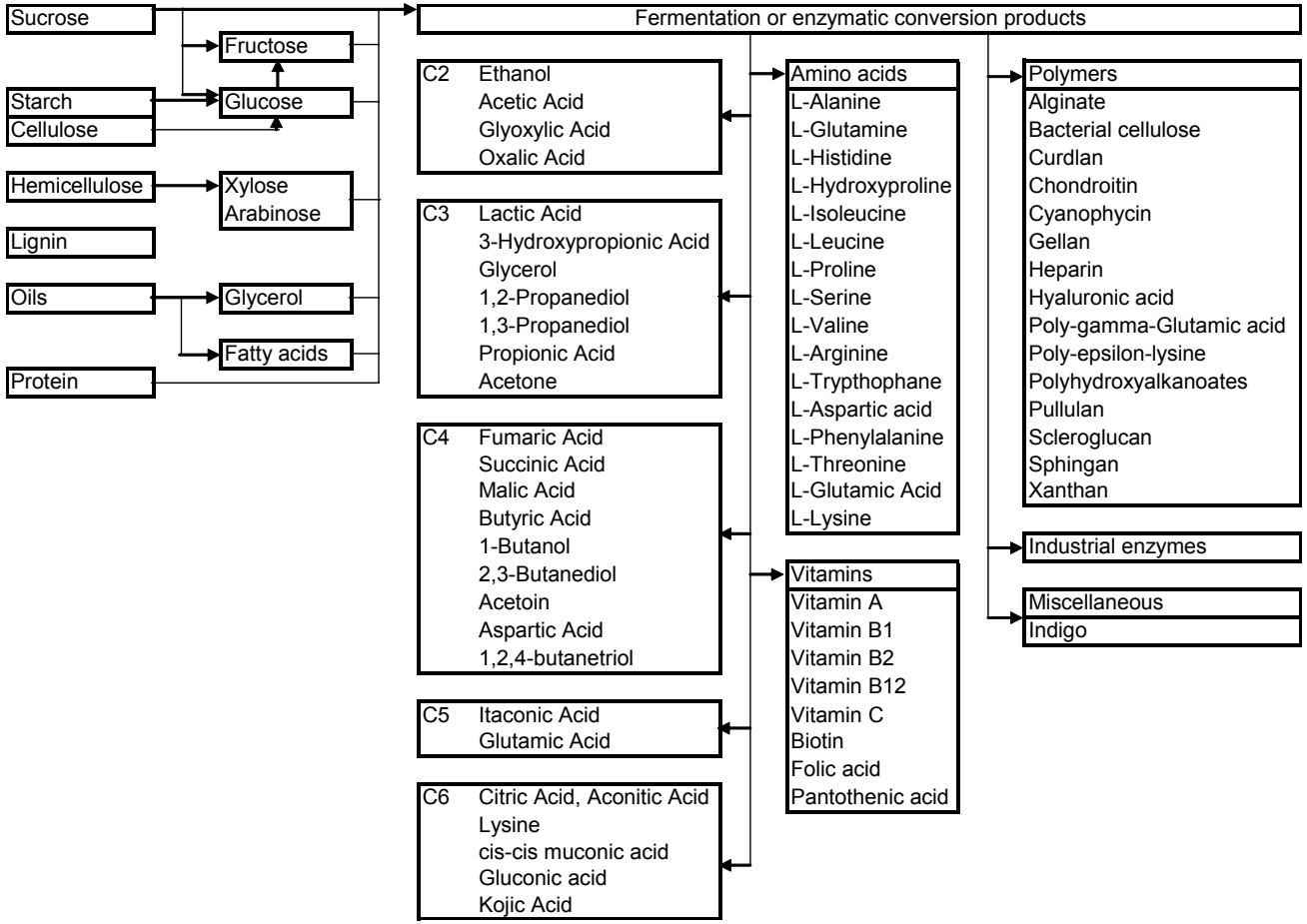

Figure 2-1: Overview of chemicals that can be obtained from major biomass constituents by established or possible biotechnological processes

Products and processes excluded from the analysis

Several industrially relevant products and processes were excluded from the analysis although they may be operated on a large scale commercially and may target major markets. They are excluded from the scope of the BREW project because their major use is in the food or feed sector, the pharmaceuticals sector, or the fine and speciality chemicals sector, or they are produced with the help of biotechnological processes or process steps from fossil resources. Table 2-1 gives an overview of these product groups.

Antibiotics
Vitamins
Amino acids (except aspartic acid, lysine, glutamic acid)
Fine chemicals
Industrial enzymes
Polymers obtained by direct modification of biomass polymers (e.g. modified starches, cellulose derivatives, chitin derivatives)

Table 2-1: Overview of product groups excluded from the analysis

2.1 C_2 building blocks

2.1.1 Ethanol

Production of ethanol

Ethanol is an interesting platform chemical because it is already today produced from biomass in bulk quantities by fermentation. In 2003, world ethanol production was estimated at approximately 40 bln l (l = litre; equivalent to approx. 31.5 million tonnes) (Berg 2004; Law 2003), with Brazil and the USA being the largest producers (approx. 14 bln l and 11 bln l production respectively). Nowadays less than 10%% of the world ethanol production was produced by chemical synthesis starting from crude oil or gas and coal, while more than 90% was derived from fermentation, using agricultural biomass as feedstock (Berg 2004; Weissermel and Arpe, 2003). Fermentation and synthetic alcohol are chemically identical. The fermentative ethanol production is dominated by large companies which make use of economies of scale. The largest producer worldwide, Archer Daniel Midlands (USA) has a production capacity of 3.4 bln l (2001), which corresponds to approximately 10% of the world ethanol production. Main producers of synthetic ethanol are only few, mostly multi-national companies, such as Sasol (South Africa, Germany), SADAF (Saudi Arabia, a 50:50 joint venture between Shell (UK, NL) and the Saudi Arabian Basic Industries Corporation), BP (UK), and Equistar (US) (Schmitz 2003).

The state of the art of biotechnical ethanol production is the large-scale fermentation of sugars or starch by yeasts, and the purification of the resulting ethanol by distillation (Wheals et al. 1999; Schmitz, 2003; Schmitz, 2005). In 2003, 61% of the world ethanol production were produced from sugar crops (sugar beet, sugar cane) or starch crops (grains, especially maize or corn is the dominating feedstock). The raw feedstocks material accounts for around 70 to 80% of the overall costs of (fuel) ethanol and therefore crucially determines the profitability of ethanol production.

This basic form of ethanol production has been gradually improved over decades and can be considered as technically mature. In order to optimise the entire process, the following process steps have to be optimised:

- Choice of substrate
- Choice of production organism
- Conditioning of substrate
- Conversion of carbohydrates to fermentable monomeric sugars
- Fermentative conversion of sugars to ethanol
- Downstream processing of ethanol
- Use of by-products and waste products of ethanol production
- Integration into overall facility concept and design, logistics

Progress in recent years has resulted in a high performance of fermentative ethanol production from sugar cane and corn (see Table 2-2). Table 2-3 to 2-7 give an overview of the state of the art in each of these steps in bioethanol production, the critical success factors/requirements, challenges and strategies to overcome bottlenecks.

For a commercially viable process, the ethanol yield (calculated as share of fermentable sugar input) must reach 90-95% of theory, and production rates of 1 g ethanol/l/h should be achieved (Zaldivar et al. 2001, p. 23).

Due to incremental process improvements, production costs for ethanol from starch declined from 0.95 US$/l ethanol in 1980 to 0.32 US$/l ethanol in 1993 (Wyman 1994, p. 11). Present production costs are estimated at 0.31-0.38 US$/l ethanol (Wooley et al. 1999, p. 801). Ethanol production costs from sugar cane in Brazil amounted to 0.26 US$/l ethanol in 1998 (Zanin et al. 2000, p. 1155). Despite these obvious improvements, even under favourable conditions bioethanol production is currently more costly than gasoline production.

	Sugar cane	Maize
Yield of crop (t/ha)	80-100	12
Sugar yield (t/ha)	12-15	n.a.
Maximum ethanol yield[6] (litre/ha)	9000	4400
Average ethanol yield[7] (litre/ha)	7750	2750
Average fermentation efficiency (%)	92	89
Typical fermentation time (h)	6-10	40
Ethanol concentration (g/l)	100	100
Ethanol productivity (g/l/h)	2	4-8

Table 2-2: State-of-the-art characteristics of ethanol production from sugar cane and corn (Wheals et al. 1999; Vogelbusch, 2006)

Note: Data on concentration and productivity refer to a continuous plant without cell recycle (lower bound) and with cell recycle (upper bound). These data originate from Vogelbusch (2006), all other data were taken from Wheals et al. (1999).

Although fermentative ethanol production is technologically mature, there are still potentials for production cost reductions. Exploiting these potentials might lead to bioethanol production costs being competitive with fuels from fossil feedstocks. Potentials for the reduction of production costs are given in (Rosillo-Calle et al. 1998; Wheals et al. 1999; Zanin et al. 2000; Zaldivar et al. 2001; Hüsing et al. 2003; Schmitz 2003):

- Implementation of modern process technology, automation and process regulation,
- Improving the energy balance by optimising energy efficiency in all process steps, but especially in downstream processing,
- Increased use of by-products, conversion to higher-value products, more energy-efficient processes for co- and waste products processing,
- Use of lignocellulosic substrates as cheaper feedstock than sugar and starch,
- Increasing ethanol yield by reducing the formation of the by-products glycerine and succinate,
- Prevention of contaminations of the production process,
- Reducing the number of process steps,
- Substrate diversification to allow for all-year ethanol fermentation.

A key focus of international research in recent years was directed to the use of lignocellulosic substrates. Within this strategy, the following challenges have to be addressed:

- *Cost-efficient, complete hydrolysis of lignocellulosic feedstock to fermentable sugars without formation of inhibitory substances*. To make fermentable sugars available, a combination of mechanical, acid and cellulase treatment processes is employed. In the USA, the optimisation of the cellulase hydrolysis is studied in several large research projects. The aim is to improve cellulase activity and/or decrease cellulase

[7] Ethanol density: 0.79 kg/l ethanol (= 1.266 l/kg ethanol).

production costs by a factor of 10. Research is also carried out on simultaneous saccharification and fermentation processes where cellulose hydrolysis and ethanol fermentation take place simultaneously. One approach within this strategy is the genetic engineering of cellulases into ethanol producers (van Wyk 2001). Weak acids, furan derivatives and phenolic substances act as inhibitors. For detoxification, treatment with laccases, chemical precipitation and extraction or ion exchange are being considered. Moreover, production strains with high tolerance towards these inhibitors and process design options (e.g. fed-batch) are being tested (Luo et al. 2001; Palmqvist et al. 2000b; Palmqvist et al. 2000a; Himmel et al. 1999).

- *Complete fermentative conversion of all sugars (hexoses and pentoses) to ethanol in a single stage*. As no naturally occurring organism is known which fulfills all requirements, one approach is to test mixed cultures of appropriate microorganisms, another, to genetically engineer good production strains (Aristidou et al. 2000; Zaldivar et al. 2001). Genetic modification approaches aim at
  - broadening the substrate range of yeasts or *Zymomonas mobilis* so that they can metabolise hemicellulose sugars such as xylose or arabinose (e.g. Becker, Boles 2003),
  - improving ethanol production. Metabolic engineering is applied to microorganisms which naturally have a broad substrate range and a high tolerance of ethanol and inhibitory substances. The aim is to confer high ethanol productivity to these organisms.

Research is underway to develop solutions to all these problems. However, an additional challenge will be to integrate all partial solutions into an overall process. It is likely that several rounds of optimisation will be required until a technical and economically competitive fermentative process, based on lignocellulosic biomass, can be established.

Several large-scale bioethanol plants are in operation now. For example, since 2003, China is home to the world's largest fuel ethanol plant. The Jilin Tianhe Ethanol Distillery has an initial capacity of 600,000 tonnes per year or 2.5 mln litres per day. Whether the final capacity can be raised to 800,000 tonnes per year (Berg 2004) remains to be seen, because there should be an optimum due to transport costs. Moreover, cleaner production technologies are being assessed and implemented in the Chinese bioethanol industry (Guo et al. 2006).

Step	State of the art	Critical success factors, requirements	Challenges	Strategies, approaches
Choice of substrate	Sugar or starch substrates from sugar cane, sugar beet, grains (especially corn, but also wheat, rye, rice); to a limited extent potatoes	Extensive experience with agricultural production; Established or imminent large-scale crop production; High and reproducible yields (productivity per area, net energy yield); Low feedstock costs (account for 70 to 80% of the overall costs of bioethanol and therefore crucially determine the profitability of bioethanol production); Lignocellulosic substrates	Experience with agricultural production of alternative crops (e.g. sweet sorghum, beets, topinambur, chicoree) not sufficient in EU for large-scale application; Lignocellulosic biomass cheap and abundant, but technically (still too) challenging	Breeding of improved crop varieties; Improving agricultural practices; Use of lignocellulosic substrates

Table 2-3: State of the art of choice of substrate in ethanol production

Step	State of the art	Critical success factors, requirements	Challenges	Strategies, approaches
Choice of production organism	Yeast, specifically adapted to industrial production process through selection	Required properties: High ethanol yield High production rates High productivity Broad substrate range (especially for use of lignocellulosic feedstocks) High ethanol tolerance High tolerance of inhibitory substances from substrate Low costs for separation from fermentation broth and disposal, closed loop systems especially for large-scale production	Naturally occuring organisms do not have all required properties; Alternative production organisms (e.g. *Zymomonas mobilis,* various clostridia) industrially not applied; Specifically designed, genetically modified organisms available, but industrially not relevant	Mixed cultures of suitable microorganisms; Genetic and metabolic engineering of production organisms to improve relevant properties; Thermophilic or thermotolerant production strains

Table 2-4: State of the art of choice of production organism in ethanol production

Step	State of the art	Critical success factors, requirements	Challenges	Strategies, approaches
Conditioning of substrate	Process depending on chosen substrate; comprises Harvest, Cutting, grinding Isolation of sugar and starch by conventional industrial techniques	High yield Cost-efficient and energy-efficient process Preventing the formation of inhibitory substances	Development of processes for lignocellulosic substrates	Improved process technology For lignocellulosics: Combination of mechanical, chemical and enzymatic treatment
Conversion of carbohydrates to fermentable sugars	In case of starchy substrates: Enzymatic conversion of starch to sugars	High yield Cost-efficient and energy-efficient process	Conversion of lignocellulosic substrates	Optimisation of cellulases (activity, production costs, production-relevant properties); Conferring high cellulase activity to ethanol producers through genetic engineering; Conferring high ethanol production ability to cellulolytic organisms (e.g. Erwinia) through metabolic engineering; Saccharication and fermentation simultaneously in one stage

Table 2-5: State of the art of conditioning of substrate and its conversion to fermentable sugars in ethanol production

Step	State of the art	Critical success factors, requirements	Challenges	Strategies, approaches
Fermentation of sugars to ethanol	Brazil: Batch-fermentations (capacity of up to 1.5 million L ethanol/day; fermentation time 9 hours, cell density 8-17%, final ethanol concentration 8-11%, yield 91.5%), recycling of production strain "Continuous" variant: series of 4-5 batch fermentations Fed-batch processes True continuous processes industrially not applied USA: broad variety of processes (batch without cell recycling to semicontinous processes and simultaneous saccharification and fermentation) Partly high level of automation, sophisticated process monitoring and control	High yields Low production costs, high energy efficiency High process stability, reliability and reproducibility	see critical success factors Prevention of bacterial contaminations; For lignocellulosic substrates: complete utilisation of all sugars (hexoses and pentoses), effects of inhibitory substances less by-products (glycerine, succinate; up to 10% of fermentable sugar)	Cutting edge process technology Optimisation of production strains (see Table 2-4)

Table 2-6: State of the art of fermentation of sugars to ethanol

Step	State of the art	Critical success factors, requirements	Challenges	Strategies, approaches
Separation and purification of ethanol	Separation of yeast by centrifugation or flocculation; Distillation of ethanol (azeotropic mixture), molecular sieve treatment	Cost- and energy-efficient separation and distillation processes	Improving the energy balance of the separation process	Energy-efficient distillation processes; Flocculating yeasts
Use of by- and waste products	Surplus biomass as animal feed, fertiliser; Energetic use of lignin (in case of lignocellulosic biomass)	High-value use; Recycling; Environmental-friendly disposal.	High-value use, recycling or disposal of large amounts of by- and waste products such as chemicals as process aids, fermentation biomass, wastewater and sludges, glycerine and succinate, Lignins	Recycling of chemicals, biomass and water; Wastewater treatment; High-value uses of biomass; Energetic and high-value use of lignins
Integration into overall facility concept and design, logistics		Improvements along the whole process chain; Closing of cycles; Exploiting economies of scale	Improvements along the whole process chain; Integrated concepts with full optimisation of all process steps in an integrated manner	Several demonstration plants for use of lignocellulosic biomass in operation

Table 2-7: State of the art of separation and purification, use of by- and waste products, and overall integration into production concept in ethanol production

Use of ethanol

There are three major uses for ethanol (Falbe, Regnitz 1989; Schmitz 2003; Weissermel, Arpe 1998; Wheals et al. 1999, see also Table 2-8):

- in the food industry (10%) as ingredient of alcoholic drinks, disinfectant and preserving agent,
- in the chemical-technical sector (21%) as solvent and as a building block for chemical synthesis and
- as fuel and fuel additive (69%)

The future development of the world ethanol market depends to a large extent on its future use as a fuel or fuel additive. This ethanol market sector is already the largest segment (2003: 28 bn l), and the most dynamically growing one due to the main drivers:

- Implementation of biofuel programmes and expansion of production capacities, due to growing political support for bioethanol. In the EU, the main drivers will be two biofuel directives by the European Commission.[8]
- Agricultural policy (use of agricultural surplusses, development of rural areas), climate and energy policy, in some countries also balance of trade considerations.

Taking into account implemented and announced policy measures to increase fuel ethanol use, and assuming (quite optimistically) that they will be realised as planned, worldwide ethanol fuel use could increase to 43 bn l in 2006 and 65 bn l in 2012 (Berg 2004). This increase in production and use is expected to go along with an ever wider geographical spread (in 2003 13 countries used ethanol as fuel or fuel additive). As a fuel additive (anti-knock agent), ethanol competes with methanol, Methyl-*tert*-butylether (MTBE) and the (ethanol-derived) ethyl-*tert*-butylether (ETBE). ETBE is chemically synthetised from ethanol (47%) and isobuten (53%). At present the world wide production of ETBE is estimated at 5 bln l (Schmitz 2003).

The future development of the world fuel ethanol market is primarily a political decision because the production costs for fuel ethanol are higher than for an equivalent amount of fossil fuels. Therefore, significant economic incentives (e.g. tax exemptions, support of investments, cheap loans) are required to make fuel ethanol commercially viable (Zaldivar et al. 2001, p. 18; Schmitz 2003; Berg 2004).

[8] The first directive, which is promotional in nature, has been approved in May 2003. Member states will now have to try to achieve a 2 % share of renewables by the end of 2005 and a 5.75 % share by the end of 2010. As a basis for reference, the energy content of all gasoline for transport placed on the market will be used. The second directive relevant for biofuels is the one on taxation of energy products. Under this directive member states will be able to exempt biofuels, such as ethanol, from the tax on mineral oil products (Berg 2004).

Ethanol use	Ethanol use in 2003 (bln l)	Share of world prod. (%)	Use description and market trends
Beverage	4	10	Component of alcoholic beverages for human consumption; Only fermentation-derived ethanol; Demand for distilled spirits in most developed countries is stagnating or even declining, due to increased health awareness.
Industrial use	8	21	Most important segment within industrial use is use as solvent (e.g. for fat, oil, resins, varnish, pharmaceuticals, adhesives), as disinfectant, preserving agent and building block for the chemical synthesis; Segment with significant market share of synthetic ethanol, competition with bioethanol depends to a large extent on feedstock prices (ethylene vs. molasses/grain); Rather modest rate of growth which is similar to the increase in Gross Domestic Product
Fuel	28	69	Substitution of gasoline only in dedicated internal combustion engines (presently only in Brazil); Use as fuel additive (anti-knock agent) in blends with gasoline (blends of 5 to 30%) or diesel (up to 3%, for higher blends special emulsifiers are needed. Competes as fuel additive with methanol, methyl-tert-butylether (MTBE) und ethyl-tert-butylether (ETBE). Used in 13 countries as a fuel component (2003); Mainly fermentation ethanol; Significant increase likely, because (sometimes ambitious) fuel ethanol programs have been proposed and may be implemented in the coming years (Optimistic estimation: 65 bn l by 2012)
Total	40	100	

Table 2-8: Overview of major ethanol uses (2003) (Falbe, Regnitz 1989; Schmitz 2003; Weissermel, Arpe 1998; Wheals et al. 1999, Berg 2004)

The industrial use of ethanol is the only area where synthetic ethanol producers hold significant market shares. While the growth of industrial use has been moderate and follows the Gross Domestic Product development, substantial future growth could be expected if both fermentatively derived ethanol and acetic acid could be used to synthesise bulk polymers and other basic chemicals from biomass resources instead of fossil feedstocks (Table 2-9). This makes these substances interesting platform chemicals. In this context it is interesting to note that companies that are moving into the renewables to chemicals market such as Cargill are already involved in ethanol production (Linton, Nisbet 2000, p. 29).

Derivative	World Production (t/a)	Route from ethanol to derivative; current status	Challenges	Main uses, market drivers
Ethylene	94 × 10^6 t (2002)	a) Steam cracking of hydrocarbons (e.g. naphtha) Established, technically mature, used on large commercial scale b) dehydration of ethanol from biomass not cost-competitive with fossil-derived ethylene	Lower production costs for ethanol Improvement of catalysts for ethanol dehydration	Replacement of fossil-derived ethylene by bio-based ethylene from ethanol. Ethylene has no direct end uses, being used almost exclusively as a chemical building block. Industrially important derivatives are polyethylene; Ethylene dichloride and polyvinylchloride; Ethylene oxide, ethylene glycols and their polymers; Acetaldehyde, and its derivatives butanol and butyraldehyde, leading to phthalates
ETBE	5 bn litres	Chemical synthesis from ethanol (47%) and isobuten (53 %) commercialised		Used as a fuel additive (anti-knock agent) ETBE competes with ethanol, and methyl-*tert*-butylether (MTBE) Main drivers: Implementation of biofuel programmes,[9] agricultural policy, climate and energy policy, in some countries also balance of trade considerations.
Ethylesters, such as ethyl acetate, ethyl lactate, ethylacrylate	1 million t/a (ethyl acetate)	Esterification of ethanol with organic acids in batch or continuous processes; final ester yield up to 95%; commercialised		Market trend: shift from aromatic and aliphatic hydrocarbons to oxygen-containing solvents because the latter have a lower ozone formation potential and better dissolution properties; demand for "green solvents"; potential to be completely derived from fermentatively produced building blocks (ethanol, acetic acid, lactic acid).

Table 2-9: Key characteristics of the routes from ethanol to its derivatives

[9] Drivers are the two biofuel directives by the European Commission The first directive, which is promotional in nature, has been approved in May 2003. Member states will now have to try to achieve a 2 % share of renewables by the end of 2005 and a 5.75 % share by end 2010. As a basis for reference, the energy content of all gasoline for transport placed on the market will be used. The second directive relevant for biofuels is the one on taxation of energy products. Under this directive member states will be able to exempt biofuels, such as ethanol, from the tax on mineral oil products (Berg 2004).

Derivative	World Production (t/a)	Route from ethanol to derivative; current status	Challenges	Main uses, market drivers
Ethylethers		commercialised		
Glycolethers		commercialised		
Ethylamine and –amide	80,000 t/a	commercialised		e.g. herbicide production
Acetaldehyde and acetic acid	1.35 million t in 1993 (acetaldehyde) 7 million t (acetate)	Oxidation of ethanol and others; commercialised	Ethanol competes as substrate with acetylene, ethylene, lower hydrocarbons, carbon monoxide and hydrogen, methanol	Main single uses of acetaldehyde are production of acetic acid and acetic anhydride, of acetate esters, of pyridine and pyridine bases

Table 2-9 continued: Key characteristics of the routes from ethanol to its derivatives

2.1.2 Acetic acid

Production of acetic acid

The total annual production of acetic acid exceeds 7×10^6 t/a. The bulk amount is synthesised by carbonylation of methanol (Cheung et al. 2000). Only 190,000 t are produced by fermentation with microorganisms, and are used for food purposes. Vinegar, an aqueous solution containing about 4–12% acetic acid, is produced by the fermentation of wine and has been known for more than 5000 years. Today, it is still made by fermentation. Ethanol and sucrose are the primary feedstocks for the microbial production of acetic acid, but biomass has also been proposed. The concentration of acetic acid in solution is limited by the ability of bacteria to survive in low-pH solutions. Consequently, research focusses on improving acetic acid productivity and improving pH tolerance of the production strains. Mutant strains of *Clostridium thermoaceticum* have been developed which produce acetic acid in solutions below pH 5. Improvement of acetic acid productivity of an *Acetobacter aceti* strain was achieved by amplification of the aldehyde dehydrogenase gene with a multicopy vector. Although bacterial production is gaining interest since it is a environmentally friendly process, cost-effective acetic acid concentration and purification remain a challenge (Cheung et al. 2000).

Use of acetic acid

The largest end uses for acetic acid are the manufacture of vinyl acetate and the production of purified terephthalic acid where acetic acid is used as a solvent. Table 2-10 gives an overview of acetic acid derivatives.

Derivative	World production (t/year)	Route from acetic acid to derivative	Main uses, drivers
Acetic anhydride	1 to 2 $\times 10^6$t	a) ketene process b) carbonylation of methyl acetate (Halcon process)	Used mainly as acetylating and dehydrating agent, e.g. for the production of acetate esters of alcohols
Vinyl acetate	4.1×10^6 t/a (2002)	Reaction of ethylene with acetic acid and oxygen in the gas phase on heterogeneous catalysts containing palladium	Vinyl acetate is used mainly for the production of polymers and copolymers; e.g. polyvinylacetate, polyvinylalcohol, ethylene-vinyl acetate copolymer, ethylene-vinyl alcohol resins
Ethyl acetate	1 million t/a	Esterification of ethanol and acetic acid	"Green" solvent
Chloroacetic acid	370,000 t/a		
Acetate salts			
Peracetic acid	18,000 t/a	Reaction of acetic acid (or acetic anhydride, acetic acid chloride) with hydrogen peroxide	Production of epoxides

Table 2-10: Derivatives of acetic acid

2.2 C_3 building blocks

2.2.1 Lactic Acid

Production of lactic acid

Lactic acid, 2-hydroxypropionic acid, $CH_3CH(OH)COOH$, is the simplest hydroxycarboxylic acid with an asymmetrical carbon atom. It is both an alcohol and an acid. It is found as a racemate (DL) and as the two optically active forms (D and L). *Synthetically* produced lactic acid is optically inactive, i.e., a racemic mixture. Lactic acid produced by *fermentation* is typically optically active. Targetted production of optically active lactic acid, whether L (+) or D (–), can be realized by using an appropriate bacterial or fungal strain (see below).

The world production of lactic acid amounted to 120,000 to 150,000 t in 2002. Moreover, 50,000 to 80,000 t of lactic acid salts and esters were produced. Major lactic acid producers are PURAC (Brazil, the Netherlands and Spain), NatureWorks LLC (USA), Archer Daniels Midland Company (USA), PGLA-1 (USA) and Galactic (Belgium).

Nearly the entire world production of lactic acid is produced on an industrial scale by *fermentation*. Only one Japanese company (Musashino Chemical Laboratory Ltd.) currently uses the synthetic route (reaction of acetaldehyde with hydrogen cyanide followed by the hydrolysis of the resulting lactonitrile) to produce racemic lactic acid. The fermentation approach has become more successful because of the lower production costs, the optical purity of the resulting lactic acid, and the increasing market demand for bio-based lactic acid.

Two different types of lactic acid fermentation exist: *homolactic* (pure lactic) fermentation and *heterolactic* (mixed lactic) fermentation. *Homolactic fermentation* produces predominantly lactic acid (either in the form of L (+) or racemic lactic acid), while *heterolactic fermentation* produces, in addition to either racemic lactic acid or D (-) lactic acid, also large amounts of other fermentation products, such as acetic acid, ethanol, formic acid and carbon dioxide. The choice of production organism determines whether a homolactic or a heterolactic fermentation occurs. In both types of fermentation, the L (+) : D (–) lactic acid ratio is influenced by the pH.

Product concentrations in commercial fermentations go up to 160 to 180 g/l with lactic acid yields above 90% of fermentable sugars. Production strains with production rates of > 5 g/l/h are available. The highest values reported in the literature are lactic acid concentrations of 771 g/l, achieved by continuous lactic acid extraction during

fermentation, and maximum production rates of 52-144 g/l/h, achieved by cell recycling (Hofvendahl, Hahn-Hägerdal 2000). Critical success factors are

- *Suitable production strain* (homo-, heterofermentative lactobacteria). Thermophilic homofermentative lactobacteria are advantageous for the following reasons: high production rates, higher calcium lactate solubility, and reduced risk of contamination with heterofermentative lactobacteria.
- *Carbon source*. Usually, glucose or molasses, sucrose or starch hydrolysates are used. It is a challenge to use other carbon sources (e.g. whole corn cobs, lignocellulosic substrates, whey) on an industrial scale. Lab to pilot scale processes have been established.
- *Nutrients*. Lactobacteria usually require complex nutrients (peptones, yeast extracts, vitamins).
- *Cell recycling and immobilisation*. In order to achieve higher cell densities and thus higher productivities, cell recycling with cell densities of 50-100 g/l proved successful, but not cell immobilisation (Hofvendahl, Hahn-Hägerdal 2000).
- *pH*. The pH is particularly important and must be maintained between 5.5 and 6.5 using neutralizing agents. Recovery of lactic acid usually generates large amounts of by-products such as calcium, sodium or ammonium sulfate. Options for use of these by-products are soil amendment/improver, use as fertilizer and wallboard production. In order to reduce the generation of these by-products, commercial lactic acid fermentations are being developed which are carried out under more acidic conditions.
- *Avoiding contaminations*. Especially lactic acid production by homofermentative lactobacteria can be contaminated with heterofermentative lactobacteria. Use of thermophilic homofermentative lactobacteria is – among other reasons – therefore advantageous.

Use of lactic acid

Main uses of lactic acid, its salts and esters in 2002 were food and beverages (97,000 t or 48%), followed by industrial applications (79,000 t or 39%) and pharmaceuticals and personal care products (26,000 t or 13%) (Bizzari, Kishi 2003, p.5). Market growth in the industrial applications segment is expected to result primarily from lactic acid based biodegradable polymers (PLA) and lactate solvents.

Derivative	World production (t/year)	Route from lactic acid to derivative	Main uses, drivers
Polylactic acid	approx. 140,000 *)	Lactic acid – Cyclic lactide – Ring-opening Polymerisation to Polylactic acid; Commercialised; Esterfication of lactide with alcohols	Applications: food and non food packaging, films, bottles and fibers. Drivers: based on renewable raw materials, technical properties and new waste disposal options such as compostability.
Lactic acid salts and esters	approx. 250,000 *)		
Lactate esters; e.g. ethyl lactate	5,000	Esterification of lactic acid with alcohols in batch or continuous processes; Final ester yield up to 95%; Commercialised	"Green solvent" for microelectronic, coating and cleaning industry Market trend: shift from aromatic and aliphatic hydrocarbons to oxygen-containing solvents because the latter have a lower ozone formation potential and better dissolution properties; demand for "green solvents"; potential to be completely derived from fermentatively produced building blocks (ethanol, lactic acid) Large market potential as costs decrease
Chiral lactate esters		Esterification with alcohols	Chiral synthons; e.g. for production of the herbicide R(+)phenoxypropionic acid
Acetaldehyde		Decarboxylation	
Acrylic acid	> $2x10^6$ t (route a)	a) Chemical synthesis from fossil resources b) Dehydration	Potential to substitute members of fossil-based acrylic acid family by bio-based ones (e.g. acrylates, polyacrylates, acrylamide)
Lactamides			Use as plasticizers
1,2-propanediol	$9×10^5$ t (1990)	a) Esterification of lactic acid, followed by hydrogenation b) Fermentative production from sugars	Important intermediate for production of propylene oxide; used in manufacture of unsaturated polyester resins (45% of propylene glycol use), of polyetherpolyols and polyurethans use as deicer and automotive antifreeze component
Propionic acid	130,000 (1989)	Reduction of lactic acid	
2,3-pentadione		Condensation	
Oxalic acid	124,000	Oxidation, decarboxylation	
Pyruvic acid		Oxidation	

*) Capacity data (not production)

Table 2-11: Derivatives of lactic acid

2.2.2 Glycerol

Production of glycerol

Glycerol, $C_3H_8O_3$, 1,2,3-propanetriol, commonly known as glycerin, is the simplest triol. It can be found in all natural fats and oils as fatty esters (see also Section 2.6). Several routes are available for the production of glycerol:

- *Synthetic glycerol from propylene*. Propylene is converted to glycerol via the intermediate stages allyl chloride and epichlorohydrin. Approximately 10% of the world production of glycerol are synthetic glycerol, with decreasing tendency.
- *Glycerol as a byproduct of splitting fats and oils* (the conversion of fats and oils to fatty acids or fatty acid methyl esters). This type of glycerol is known as natural or native glycerol, in contrast to synthetic glycerol from propylene. For the manufacture of fatty acids on a commercial scale, only fats available in large quantities are used as raw materials. Fats are fatty acid esters of glycerol and are also known as triglycerides. By splitting the glycerides, fatty acids and glycerol can be recovered. The most important splitting agents are water (hydrolysis), methanol (methanolysis), caustic soda (saponification), and amines (aminolysis). Because of drawbacks in the subsequent purification of glycerol, saponification and aminolysis are no longer commercially important. Bio-based glycerol today is mainly produced by high-pressure splitting and transesterification. In High-Pressure Splitting water and fat are fed into continuous process reactors at 2 – 6 MPa and 220 – 260 °C, leading to a approx. 15% solution of glycerol in water, known as sweet water. This glycerol is marketed as 88% saponification- or hydrolysis-crude glycerol. By means of transesterification, oils and fats are converted to their methyl esters. Continuous processes are dominating. Glycerol from the low pressure transesterification process has a much higher salt content of 2 – 5%. The crude glycerol is obtained directly at a concentration of approx. 90 – 92%. Economics of oleochemical processes are to a large extent determined by the cost of glycerol which is an inevitable by-product of the conversion of natural fats and oils to derivatives. In particular, the very strong production increase of rapeseed methyl ester (RME), which is sold as biodiesel, has led to large by-production of glycerol. Given that glycerol accounts for approximately 10% of the biodiesel output (approx. 1.3 million t produced in Europe in 2003 and approx. 3.4 million t in 2005), the production from this source has added 100-300 kt, representing around 15% to up to 40% of the global glycerol market. As a consequence, the spot prices for glycerol have dropped from around 1450 US$/t to less than 1000 US$/t. This makes glycerol increasingly attractive as raw material of chemical synthesis and as feedstock for biotechnological processes.

- *Enzymatic splitting of fats and oils with lipases*. Not industrially important; only employed for speciality products.
- *Fermentation of sugar*. Not industrially important.

- *Hydrogenation of carbohydrates*. Not industrially important. Hydrogenation of natural polyalcohols such as cellulose, starch, or sugar leads to mixtures of glycerol and glycols, which can be separated by distillation. Catalysts used in this high-temperature reaction include nickel, copper, cobalt, chromium, and tungsten, as well as oxides of some of the lanthanides.

Total production is estimated at approx. 750 000 t/a (1998); about 90% is produced by processing of natural oils or fats and 10% - with decreasing tendency - is synthesized from propylene. An increasing amount is produced as by-product of the rapeseed methyl ester production (RME; approx. 10%).

Use of glycerol

The economics of oleochemical processes are to a large extent determined by the cost of glycerol which is an inevitable by-product of the conversion of natural fats and oils to derivatives. There is a need for new and high-value uses of glycerol in order to make oleochemical reactions economically attractive, and to use the increasing amounts of glycerol which become available as by-product from RME production.

Glycerol is a reactive molecule that undergoes all the usual reactions of alcohols. Its possible uses comprise

- *Esters, mono-, di-, and triesters of inorganic and organic acids*. Glycerol forms esters with both inorganic and organic acids; depending on reaction conditions and the degree of esterification, these can be mono-, di-, or triglycerides. Of most importance are esters produced from nitric, acetic, and fatty acids.
  - *Glycerol trinitrate,* nitroglycerin, is produced in a mixture of nitric and sulfuric acids. It is used as an explosive and pharmaceutical.
  - The *acetins* are produced industrially by esterification of glycerol with acetic acid, acetic anhydride, or both. They are the most important esters of glycerol from short-chain carboxylic acids. The most widely used type of acetin is triacetin.
  - *Glycerol fatty esters,* the partial glycerides, mono- and diglycerides of fatty acids formed by transesterification of triglycerides (from fats) are obtained by transesterification of fats or oils with glycerol to a mixture of mono- and diglycerides. The mono- and diesters of fatty acids are edible, as are the triglycerides.
  - *Aliphatic and aromatic esters*, formed by reaction with alkylating or arylating agents, respectively.
- *Oxidations*. Glycerol is easily oxidized: the terminal carbon atoms to aldehyde or carboxyl groups and the central carbon atom to a carbonyl group. Biochemical oxidation of glycerol has also been described.
- *Cyclic 1,2- or 1,3-acetals or ketals*, formed by reaction with aldehydes or ketones, respectively.
- *Glycerol polyoxyalkylenes*, formed by alkoxylation of glycerol(s) with ethylene- or propylene oxide under alkaline conditions.

- *Polyglycerols*. At 180 °C, alkaline glycerol begins to dehydrate, forming ether-linked polyglycerols. However, the process is difficult to control so that a wide range of different polyglycerols results. Another option is the reaction of glycerol and epichlorohydrin with consecutive alkaline hydrolysis or by intermolecular elimination of water with alkaline catalysts (diglycerol). Possible uses of polyglycerols are non-ionic surfactants. Diglycerol esters are mainly used as emulsifiers in food, cosmetics and some technical applications, as well as antifogging agents in polyolefin films (Vicente et al. 2005).
- *Acrolein*. Catalytic hydrolysis of glycerol to acrolein.
- *1,3-Propanediol*. Conversion to 1,3-Propanediol, either chemically or fermentatively, and further derivatization (see also Section 2.2.4).
- *1,2-Propanediol.* Research is underway to convert glycerol to propylene glycol by hydrogenolysis (see e. g. Dasari et al. 2005).
- Epichlorohydrin. Epichlorohydrin can be produced from glycerol and hydrochloric acid which react to dichloropropanol, followed by a dehydrochlorination to epichlorohydrin. The entire process is marked by a lower specific consumption of chlorine and water, consequently reducing chlorinated effluents. This process was developed by Solvay and is named Epicerol process. The company announced in 2006 that it will use this process in a newly built epichlorohydrine plant which is expected to come operational in 2007 and will have a capacity of 10,000 t/year. The feedstock will be glycerol from biodiesel production from rapeseed oil. Epichlorohydrin is mainly used for the production of epoxy resins, paper reinforcement and water purification.[10]
- *Substrate for fermentative processes*. If glycerol becomes available at low cost, e.g. as by-product from RME production, it may become economically attractive to use it as substrate for certain fermentative processes, instead of carbohydrates. However, the effect of inhibitory substances which are abundant in these crude glycerol fractions must be overcome.
- *GTBE (glycerol tertiary butyl ether).* In analogy to MTBE, GTBE could be used as oxygen-containing additive for diesel fuels.
- *Polymers*. Use in polymers through conversion to glycerol carbonate. This can either be further reacted to dimethyl carbonate that can replace phosgene in polycarbonates and polyurethans. Glycerol carbonate can also be converted to glycidol which is then either polymerised to polyglycidol, or is used to synthesize alcohol epoxide derivatives.

[10] http://www.solvay.fr/actualites/0,,38782-2-0,00.htm

2.2.3 3-Hydroxypropionic acid

Production of 3-hydroxypropionic acid

3-hydroxypropionic acid (3-HP) is a platform intermediate that is considered to be an entry into the 1,3-difunctional space that includes malonic acid and 1,3-propanediol (PDO). 3-HP is not readily produced by chemical synthesis, but research is underway to establish a fermentative route from glucose or glycerol to 3-HP. Glycerol or glucose is first converted to 3-hydroxypropionic aldehyde (3-HPA) which is then converted to 3-HP.

For this purpose, transgenic microorganisms are constructed which simultaneously express a glycerol dehydratase gene and a gene for an aldehyde dehydrogenase which are required and sufficient for 3-HP production from glucose or glycerol (Suthers, Cameron 2001). Stochiometrically, a theoretical yield of 100% from glucose could be possible. However, a recent theoretical analysis of the bioenergetics of different export mechanisms relevant for lactic acid and 3-HP production showed that export can be a key constraint in industrial production, especially under the conditions of high product concentration and low extracellular pH that are optimal for recovery of the undissociated acids. Under these conditions, the metabolic energy requirement for product export may equal or exceed the metabolic energy yield from product formation. Consequently, prolonged product formation at low pH and at high product concentrations requires the involvement of alternative, ATP-yielding pathways to sustain growth and maintenance processes, thereby reducing the product yield on substrate. Research on export mechanisms and energetics should therefore be an integral part of the development of microbial production processes for these and other weak acids (Maris et al. 2004).

Research into 3-HP fermentative processes is carried out by Cargill. The company invests 6 million US-$ in the project over three years (2002-2005). Additional 6 million US-$ are provided by a grant from the United States Department of Energy (DOE), as part of a program to develop new technologies for producing chemicals and fuels from sustainable raw materials such as carbohydrates and oils.[11]

Up to now, the key genes for glycerol dehydratase (dhaB from *Klebsiella pneumoniae*) and for four different aldehyde dehydrogenases from various organisms (aldA and aldB from *E. coli*, ALD4 from the yeast *Saccharomyces cerevisiae*, and AKDH2 from humans) have been cloned and sequenced. Several *E. coli* strains have been constructed and were shown to produce 3-HP from glycerol, albeit in low quantities. The yeast aldehyde dehydrogenase ALD4 performed better than the other enzymes tested (Suthers, Chelf 2005). In May 2003, Cargill and Codexis Inc. announced an agreement that Codexis will use its proprietary MolecularBreeding™ directed molecular evolution

[11] http://www.cargill.com/news/news_releases/2002/021031_energy.htm

technologies to enhance 3-HP production,[12] and after achieving a key milestone in 2005, the two companies are now negotiating an extension of their existing agreement.

For 3-HP production to become commercially feasible, substantial improvements are still required. Challenges are (Werpy, Petersen 2004):

- Construction of a production strain by pathway engineering, also taking transport processes and cofactor requirement of enzymes into account,
- Improvement of productivity (goal: 2.5 g/l/h) and final titer, avoiding of side products which decrease yield,
- Low cost recovery process,
- Scale up and system integration issues.

Use of 3-hydroxypropionic acid

The basic conversions of 3-HP to industrial chemicals such as 1,3-propanediol, acrylic acid, malonic acid, and acrylamide have been demonstrated[13] (Table 2-12). Moreover, a research project is underway (2004-2005) which aims at investigating the synthesis and properties of polyesters using 3-HP as the primary building block. The project comprises the development of strategies for the preparation of biodegradable polyesters from 3-HP, the preparation and characterisation of novel copolyesters that contain 3-HP and other building blocks from renewable resource materials (e.g. lactic acid, glycolic acid), and the establishment of structure/property relationships in new 3-HP-based materials.[14]

[12] http://www.cargill.com/news/news_releases/2003/030519_codexis.htm?FILTERNAME=%40URL\&FILTERVALUE=news\&GO=%BB

[13] http://www.nrel.gov/biotechsymp25/docs/abst5-03.doc

[14] http://www1.umn.edu/iree/funded_projects_2004.html

Derivative	World production (t/year)	Route from 3-hydroxypropionic acid to derivative	Main uses, drivers
Propiolactone			
Malonic acid		Platinum group metal-catalyzed oxidation of 3-hydroxypropionic acid	
Ethyl-3-hydroxypropi-onic acid			
L-serine			
L-alanine			
1,3-propanediol (PDO)		Hydrogenation	Direct use as building block in polymers such as PTT; Synthesis of PDO derivatives: 1,3 dioxanes, ethers, polyurethans, malonic acid; Would compete with the DuPont process of producing 1,3-propanediol fermentatively from C_6 sources (Section 2.2.4)
Acrylic acid, acrylamide	> $2x10^6$ t (route a)	a) Chemical synthesis from fossil resources b) Dehydration	Potential to substitute members of fossil-based acrylic acid family by bio-based ones (e.g. acrylates, polyacrylates, acrylamide)
Comonomer in polyalkanoate polymers	-		

Table 2-12: Derivatives of 3-hydroxypropionic acid

2.2.4 1,3-Propanediol

Production of 1,3-propanediol

1,3-propanediol (PDO, 3G, 1,3-propylene glycol, trimethylene glycol) is a linear aliphatic glycol with two primary hydroxyl groups with equivalent reactivity and is an isomer of propylene glycol. After the shutdown of the *DuPont/Degussa-process* based on acrolein (via 3-hydroxypropionic aldehyde) the *Shell process* is the only petrochemical process in operation on industrial scale. : Ethylene oxide is hydroformylated to 3-hydroxypropionaldehyde (HPA), followed by hydrogenation of HPA to PDO. Shell produces PDO since 2000 at Geismar, Louisiana with a capacity of 73,000 t PDO/year[15] and presently is the largest producer of 1,3-propanediol in the world.

The annual world capacity of PDO is more than 80,000 t/year, the leading manufacturers are Shell and DuPont.

Three biotechnological processes are known for the production of PDO:

- Fermentative production from glycerol as carbon source.

[15] http://www.shellchemicals.com/locations/1,1098,42-location_id=24,02.html

- Fermentative production from glucose as carbon source in two-stage processes or by mixed cultures.
- Fermentative production from glucose as carbon source by pathway engineered microorganisms (DuPont process).

Options (1) and (3) have been intensively investigated (for recent reviews see Zeng, Biebl 2002; Nakamura, Whited 2003), with option (3) being on the verge of commercialisation, whereas for option (2) only the proof of principle has been given (Chotani et al. 2000). Therefore, option (2) will not be considered further in this section.

The fermentative production of PDO from glycerol as carbon source (option 1) is a dismutation process involving two pathways: Through one pathway, glycerol is dehydrogenated to dihydroxyacetonephosphate and funneled to glycolysis. In order to regenerate surplus NADH, glycerol is dehydrated to 3-hydroxypropionaldehyde in the second pathway, which is then reduced to 1,3-propanediol. The pathway involves four key enzymes which are encoded in the dha regulon. It is induced when dihydroxyacetone or glycerol are present. *Citrobacter freundii*, *Klebsiella pneumoniae* and *Clostridium butyricum* as well as *Clostridium pasteurianum* are natural 1,3-propanediol producers. Performance characteristics of optimised 1,3-PDO fermentations from glycerol are given in Table 2-13. Drawbacks for industrial processes employing these organisms are the strong inhibition of 1,3-propanediol production and formation of by-products during fermentation in the presence of inexpensive cosubstrates such as glucose. Research is underway to develop optimised key enzymes (Knietsch et al. 2003) and screen for better PDO producers. A major drawback for industrial use is the requirement for the – up to now – relatively expensive starting material glycerol. With increasing availability of glycerol due to increased biodiesel production and subsequently falling glycerol prices, 1,3-propanediol fermentations based on glycerol as carbon source could become economically more attractive than they were in the past.

Characteristics	Glycerol	Glucose
Organism	*Klebsiella pneumoniae, Clostridium butylicum*	Recombinant *E. coli*, modified in more than 10 genes
PDO concentration	80-85 g/l	135 g/l
PDO production rate	3.0 g/l/h	3.5 g/l/h
Yield (w/w)	55%	51%
Type of process	anaerobic, fed-batch	aerobic

Table 2-13: State of the art characteristics of 1,3-propanediol (PDO) production from glycerol and glucose, respectively (Menzel et al. 1997; Zeng, Biebl 2002; Nakamura, Whited 2003)

No naturally occurring microorganism is known which could produce PDO from the carbon and energy source glucose which has been – at least up to now – been much cheaper than glycerol. The company DuPont, in collaboration with Genencor and Tate & Lyle, has since 1995 developed a recombinant production organism as well as a fermentation process based on glucose from corn starch for the commercial production

of PDO (termed Bio-PDO^{TM}). After operating a pilot plant in Decatur, Illinois since 2000, a first commercial production plant with a PDO capacity of 45,000 t/year is under construction in Loudon, Tennessee, operated by the joint venture DuPont Tate&Lyle BioProducts LLC. The manufacturing facility for Bio-PDO^{TM} is planned to come on-stream in 2006.

The production strain is based on an *E. coli* K12 strain which has been substantially engineered in order to produce PDO from glucose (Nakamura, Whited 2003; Kurian 2005). The alterations involve

1) changing an anaerobic process to an aerobic one,
2) replacing the feedstock uptake (transport) mechanism of the host organism,
3) intergeneric transfer of complex metabolic pathways, and
4) designing and implementing an optimum solution to the balance of carbon, redox, and energy with respect to microbial growth and product formation.

In order to confer the ability to produce 1,3-PDO from glucose to *E. coli*, a new pathway was introduced. It comprises five biosynthetic genes from *Saccharomyces cerevisiae* and *Klebsiella pneumoniae*, respectively, three genes for reactivating factors of the glycerol dehydratase from *Klebsiella pneumoniae*, and one endogeneous oxidoreductase gene from *E. coli*. Moreover, gene deletions were introduced to eliminate non-productive reactions (e.g. conversion of glycerol to other products than PDO). In addition, the PEP-dependent glucose transport system of *E. coli* was replaced by a more efficient synthetic glucose uptake system, comprising galactose permease and glucokinase. Finally, the expression level of several enzymes outside of the direct carbon pathway to PDO were modulated. The resulting metabolically engineered production organism has characteristics in fed-batch 10-l-fermentations that are given in Table 2-13 (Nakamura, Whited 2003).

DuPont's recent success with 1,3-PDO could well provide stimulus to those interested in developing an commercial bioroute to BDO in order to produce bio-based PBT (polybutylene terephthalate) (Crank et al. 2005, p. 51). For BDO, refer to Section 2.3.5.

Use of 1,3-propanediol

As a diol, 1,3-propanediol is subject to many of the same polymeric applications as other low molecular mass diols (e.g., ethylene glycol, and 1,4-butanediol). At present, the main use of PDO is as co-monomer with terephthalic acid or dimethylterephthalate (DMT) for the manufacture of the polymer polytrimethylene terephthalate, PTT. These polymers have been commercialized by Shell chemicals companies under the trademark Corterra Polymers, and by DuPont under the trademark Sorona.

The world market is growing rapidly: The world production capacity for PTT in 2003 amounted to approx. 30,000 t. In late 2004, PolyCanada's[16] PTT plant with a capacity of

[16] This is a 50/50 limited partnership between Shell Chemicals Canada Ltd and Société générale de

95,000 t PTT/year came on-stream near Montreal, Canada, so that in 2005, the production capacity in 2005 well exceeds 100,000 t/year (2005). It is estimated that until 2010, the production capacity for PTT will be increased to 0.5 to 1 mill. t/year, among others through retrofitting of existing PET or PBT facilities[17] (Crank et al. 2005).

The present PTT production is completely based on fossil feedstocks. However, DuPont Tate&Lyle BioProducts LLC has announced to produce Bio-PDO™ on a commercial scale from 2006 onwards, so that the resulting PTT would comprise a bio-based PDO part.

PDO can also be used in laminates, adhesives, paints, powder and UV-cured coatings, and in inks as either a component or chemical intermediate. It can also be used as a solvent and as a coolant, and in conjunction with other monomers in the manufacture of other polymers and co-polymers (Table 2-14).

Derivative	World production (t/year)	Route from PDO to derivative	Main uses, drivers
PTT	>100,000 (installed capacity, 2005)	a) Transesterifi-cation of PDO with dimethyl terephthalate (DMT) b) Esterification of PDO with terephthalic acid (PTA)	Favourable properties of the polymer for many applications, e.g. Textiles and apparel, upholstery, carpeting Industrial fibres Engineering plastics Resins Packaging (films) High substitution potential for nylon and PET, moderate potential for PBT, PC and PP The bio-based version of Sorona® will be available to markets in 2006.
Malonic acid		Platinum group metal-catalyzed oxidation of 3-hydroxypropionic acid	
1,3 dioxanes			
Propane-1,3-diol-bis-(4-aminobenzoate)			
Polyurethans			Chain extender for thermoplastic polyurethans instead of 1,4-butanediol
Copolyester ethers			High performance elastomers

Table 2-14: Derivatives of 1,3-propanediol

financement du Québec (SGF)

[17] This strategy is currently pursued by DuPont.

2.2.5 Acrylic acid

Production of acrylic acid

Acrylic acid, 2-propenoic acid, CH_2=CHCOOH, is mainly produced by the catalytic oxidation of propylene via acrolein. The world production capacity of acrylic acid amounts to 4.2 million t/year, the world production of acrylic esters is estimated at 1.2 million t/year.

Up to now, no fermentative routes from biomass to acrylic acid have been developed (for conversion of fermentatively produced lactic acid to acrylic acid see Section 2.2.1). However, a highly speculative process has recently be designed which involves biosynthetic pathways which proceed via β-alanine, methylcitrate, or methylmalonate-CoA. Expression of this pathway in a production organism would require extensive genetic engineering in order to achieve plausible mass and redox balances, plausible biochemistry, and plausible energetics (Straathof et al. 2005).

Use of acrylic acid

The main use of acrylic acid and its esters (such as methyl, ethyl, *n*-butyl, and 2-ethylhexyl acrylates) is the production of polymers. Other esters, including multifunctional acrylates, are produced for special applications. The world production of acrylic acid amounts to 2 million t/year, the world production of acrylic esters to 1.2 million t/year.

2.3 C_4 building blocks

2.3.1 Succinic Acid

Production of succinic acid

Succinic acid (HOOC-CH_2-CH_2-COOH) is an aliphatic, saturated C_4 dicarboxylic acid. It is currently a low volume chemical, being produced in quantities of approx. 16,000 t/year. A large number of chemical syntheses are available for the manufacturing of succinic acid. Usually, it is produced by catalytic hydrogenation of petrochemically derived maleic acid or maleic anhydride.
Succinic acid can also be produced fermentatively from carbohydrates in a mixed-acid fermentation. In addition to succinic acid, ethanol, lactic acid, acetic acid, formic acid, propionic acid and other acids and alcohols are formed, their amount and share depending on the production organism and the cultivation conditions. At present, two approaches are pursued to bring fermentative succinic acid production to commercial maturity:

- *Optimisation of excellent natural succinic acid producers*. Excellent succinic acid producing organisms are e.g. *Anaerobiospirillum succiniproducens* and *Actinobacillus succinogenes*. Final succinate titers of up to 110 g/l, productivities of 1.8 g/l/h and conversion rates of 1.2 mol succinate/mol glucose have been reported (Lee et al. 1999b; Lee et al. 1999a; Tsao et al. 1999; Zeikus et al. 1999; http://www.mbi.org/programsR&D.html). Organisms which use both hexoses and pentoses as substrates have been developed (Kim et al. 2004a; DoE funded research projects; http://www.dnpco.com; http://www.mbi.org/programsR&D.html). However, conventional strain improvement does not seem to be sufficient so that metabolic engineering is also applied to improve strain productivity. This approach seems to be delayed by the lack of molecular genetic tools for these organisms. For example, the construction of a shuttle vector for *Actinobacillus succinogenes* as a prerequisite for genetic pathway engineering in this organism has only recently been reported (Kim et al. 2004b). Moreover, enzyme engineering activities of key enzymes in the synthetic pathway to succinic acid have started (Jabalquinto et al. 2004). No publications could be identified, however, on the question whether these approaches lead to improvements in strain productivity or yield.
- *Pathway engineering of Escherichia coli*. In contrast to natural succinic acid producers which employ only one major pathway for succinic acid production, *E. coli* uses a total of six biosynthetic routes. Pathway engineering is being performed in order to direct carbon flow predominantly to succinic acid, assisted by *in silico* metabolic pathway analysis of engineered strains (Lee et al. 2002). Although considerable progress has been achieved (Lin et al. in press), and final succinate titers of 50 g/l could be obtained (Chotani et al. 2000; Nghiem et al. 1998), it is

difficult to assess the significance of these approaches because engineered *E. coli* still produce significantly lower amounts of succinic acid than natural producers.

A key challenge for the coming years is the significant reduction of production costs for the fermentative production process for succinic acid in order to become competitive with succcinic acid production from maleic acid. According to DoE, production costs have been decreased from 2 US-$/pound in 1992 to 0.5 US-$/pound in 2003 (http://www.wisbiorefine.org), but have to be further reduced to or below 0.25 US-$/pound.[18] Goals and approaches are (see also Werpy, Petersen 2004, p. 24; Table 2-15):

- *Increases in productivity.* Current productivities of 1 to 2 g/l/h have to be increased to approx. 2.5 g/l/h. Moreover, production of coproducts (alcohols, acids) must be minimised. Metabolic engineering approaches are favoured in order to achieve these goals, but are delayed by a lack of tools for natural succinic acid producing organisms.
- *Increases in yield and final titers*. While yields have been achieved which are close to the theoretical maximum (95%), final titers of up to 100 g/l should still be improved in order to reduce overall separation and concentration costs.
- *Fermentation substrate.* Good production strains, originally isolated from rumen, require complex and expensive growth medium components. There is a need to develop low-cost fermentation media without these additives, and which make use of low-cost carbohydrates, such as lignocellulose hydrolysates. This requires the adaptation of production strains which are inhibited by components in such hydrolysates.
- *pH, recovery process optimization*. At present, fermentative succinic acid production requires neutralisation which adds cost to convert the resulting sodium succinate to the free acid required for subsequent derivatization. Acid-tolerant production strains could be an option to avoid the need for neutralisation.
- *Scale-up and system integration issues*.
- *Development of analogous fermentation processes for fumaric and malic acid*.

[18] 1 pound = (1 / 2.2046226) kilogramme; corresponds to 4.4 US$/kg in 1992; 1.1 US-$/kg in 2003; and 0.55 US-$/kg in the future.

Building block	World Production (million t/a)	Route from biomass to building block	Current status	Challenges	Main uses, market drivers
Succinic acid	0.015	Mixed acid fermentation of sugars by engineered microorganisms	Lab to pilot scale	- Production cost reduction from 1.1 US-$/kg to at least 0.55 US-$/kg - Increases in productivity from 1 to 2 g/l/h to approx. 2.5 g/l/h. - Minimisation of coproducts (alcohols, acids) - Implementation of metabolic engineering tools for natural succinic acid producing organisms. - Increases in yield and final titers. - Lower cost fermentation substrates. - pH considerations, recovery process optimization. - Scale-up - System integration issues. - Development of analogous fermentation processes for fumaric and malic acid	Sweetener in food and beverages; Used as feedstock for fermentations and as feedstock for (bio)chemical non-food valorisation, but potential still underexploited

Table 2-15: Key characteristics of the routes from biomass to the building block succinic acid

Use of succinic acid

The chemical behavior of the dicarboxylic acid succinic acid is determined principally by its two carboxyl groups. The following reactions and derivatives are considered interesting; additional information is given in Table 2-16:

- Reductions of succinic acid to 1,4-butanediol, γ-butyrolactone and tetrahydrofuran and their derivatives,
- Reductive amination of succinic acid or γ-butyrolactone, respectively, to pyrrolidinones,
- Polymerisation of succinic acid with diols, therefore use as building block of polyesters, e.g. polybutylene succinate (PBS),
- Succinic salts for use as coolants or deicing compounds,
- Succinate esters, e.g. diethylsuccinate, as fuel additive or "green" solvents,
- Polymerisation of succinic acid with diamines to form polyamides,
- Amidation to succindiamine, polymerisation with acids to polyamides.

To sum up, the future demand for succinic acid is price sensitive. Expansion of the market is projected to come from three areas:

- as new polymer intermediate,
- in the manufacture of butanediol, tetrahydrofuran and (-butyrolactone, and
- as an analogous replacement for maleic anhydride.

In these functions, succinic acid has the potential to create a “green" C_4 platform, provided that the production costs can be lowered to at least 0.55 US-$/kg. Similar chemical derivatizations can be applied to malic and fumaric acid, so that they can also be considered interesting C_4 building blocks.

Derivative	World Production (t/a)	Route from succinic acid to derivative; current status	Challenges	Main uses, market drivers
1,4 butanediol (BDO)	512,000 t/a in 1995	Catalytic reduction of succinic acid to 1,4-butanediol; Technically feasible	Lower production costs for succinic acid to become cost-competitive with fossil-derived BDO; Improvement of catalyst selectivity and tolerance to fermentation-derived contaminants	Replacement of fossil-derived BDO by bio-based BDO in polybutylene terephthalate, PBT. PBT production volume in 1997 was 340,000 t/year with an average growth rate above 6%. Replacement of fossil-derived building blocks by bio-based building blocks in polybutylene succinate (PBS). Present PBS production capacity is around 3,000 t/year (Showa Highpolymer); announcement of bio-based PBS production by Mitsubishi Chemical and Ajinomoto by 2006 (initial annual capacity of 30,000 t); Further conversion of BDO to tetrahydrofuran
Tetrahydrofuran (THF)	1.4×10^5 t (1992)	Catalytic reduction of succinic acid to 1,4-butanediol, followed by cyclization of BDO to THF; Technically feasible	Lower production costs for succinic acid to become cost-competitive with fossil-derived THF; Improvement of catalyst selectivity and tolerance to fermentation-derived contaminants	Replacement of fossil derived THF by bio-based THF. THF is mainly used as a solvent and as an intermediate in the production of thermoplastic polyurethanes, elastic fibers, molded elastomers, and copolyesters or copolyamides.
γ-butyrolactone (GBL)		Catalytic reduction of succinic acid to 1,4-butanediol, followed by endothermic dehydrogenation of BDO in the gas phase in the presence of copper – zinc – aluminum catalysts Technically feasible	Lower production costs for succinic acid to become cost-competitive with fossil-derived GBL; Improvement of catalyst selectivity and tolerance to fermentation-derived contaminants	Replacement of fossil derived GBL by bio-based GBL. Butyrolactone is important as an intermediate in the manufacture of pyrrolidone derivatives and as a solvent for polymers and agrochemicals.

Table 2-16: Key characteristics of the routes from succinic acid to its derivatives

Derivative	World Production (t/a)	Route from succinic acid to derivative; current status	Challenges	Main uses, market drivers
Pyrrolidinones, e.g. *N*-Methyl-2-pyrrolidone (NMP)	20,000 – 30,000 t/a (NMP)	a) Selective reductive amination of succinic acid salts b) Reductive amination of succinic anhydride c) Reduction of succinic acid to BDO, followed by reductive amination of BDO; Technically feasible	Lower production costs for succinic acid to become cost-competitive with fossil-derived pyrrolidinones; Improvement of catalyst selectivity and tolerance to fermentation-derived contaminants	Replacement of fossil derived pyrrolidinones by bio-based ones. *N*-Methyl-2-pyrrolidone (NMP) is an important, versatile solvent and reaction medium for the chemical industry.
Diethylsuccinate and analogous succinate esters		Esterification of succinic acid with alcohols; Technically feasible	Lower production costs for succinic acid to become cost-competitive with fossil-derived alternatives	Use as fuel oxygenates; drivers: environmental legislation, costs Use as green solvents with environmentally favourable properties
Polyamides based on succinic acid		Polymerisation of succinic acid with diamines	Lower production costs; Control of polymerisation; Favourable polymer properties	New polyamides
Polyesters based on succinic acid		Polymerisation of succinic acid with diols	Lower production costs; Control of polymerisation; Favourable polymer properties	New polyesters, see also above, BDO
Succinic salts	90,000 t (only US market potential)	Formation of succinate during fermentation; State of the art	Lower production costs to become cost-competitive to conventional alternatives	Use as coolants, could be alternatives to glycols; Use as airport deicing compounds with more favourable environmental properties than conventional deicers; Prevents need to develop low pH fermentations without neutralisation

Table 2-16 continued: Key characteristics of the route from succinic acid to its derivatives

2.3.2 Fumaric acid

Production of fumaric acid

Fumaric acid, *trans*-butenedioic acid, is produced on an industrial scale, starting from maleic acid or maleic anhydride: Maleic acid is converted almost quantitatively by thermal or catalytic isomerization into fumaric acid, which is recovered by filtration. Thiourea is most commonly used in practice as catalyst. The world production of fumaric acid is approx. 12,000 t/year.

Several fermentative processes for the production of fumaric acid from carbohydrate substrates (mainly glucose, molasses) with fungi (mainly *Rhizopus,* but also *Mucor, Aspergillus)* have been developed, but do not play a significant role in industrial fumaric acid production. For fumaric acid overproduction, the fungi are cultivated under growth limitation due to a low nitrogen/carbon ratio or phosphorus limitation, a high aeration rate, and in the presence of a neutralising agent (e.g. $CaCO_3$). The preferred substrates are glucose or molasses. Various low-cost carbohydrate containing substrates have also been tested. Processes utilising fats, fatty acids or fatty acid esters as carbon source additives have also been described in order to enhance the rate of production of fumaric acid. In addition to fumaric acid biosynthesis via the tricarboxylic acid cycle, a cytosolic pathway exists which converts pyruvate to fumarate by the combined activities of pyruvate carboxylase, malate dehydrogenase and fumarase, leading to high fumarate molar yield (greater than 100%). The process characteristics that are typically obtained in batch cultures are listed in Table 2-17.

Fumaric acid final concentration	12-25 g/l
$Yield_{max}$	2 mol fumaric acid/mol glucose consumed 1.29 g fumaric acid/g glucose consumed
$Yield_{typ}$	up to 1.45 mol fumaric acid/mol glucose consumed0.3 to 0.9 g fumaric acid/g glucose
Volumetric productivity	0.3 to 1.0 g fumaric acid/l h (stirred tank) 4.2 g/l/h (immobilised cells, continuous fumaric acid removal by adsorption

Table 2-17: Typical process characteristics for fumaric acid fermentations (Cao et al. 1996; Zhou et al. 2002; Carta et al. 1999; Kenealy et al. 1986; Lee et al. 2004)

Efforts to improve fumarate production seem to have focussed on process engineering (e.g. different carbon sources, aeration, immobilisation, in-situ product removal). No genetic and metabolic engineering approaches of the production organisms with a focus on fumaric acid production could be identified.

Drawbacks are low production rates and yields, the presence of other organic acids as fermentation products (e.g. succinic acid, malic acid, ketoglutaric acid), and, in case $CaCO_3$ is used as neutralising agent, the formation of gypsum that has to be disposed of. Biotechnical processes for fumaric acid production will have to compete with bioprocesses for succinic (Section 2.3.1) and aspartic acid production (Section 2.3.3).

Use of fumaric acid

The world production of fumaric acid is approx. 13,000 t/year. It is used directly as a food acidulant and beverage ingredient. Fumaric acid (Fumaril) and iron(II) fumarate are used as special additives for animal feeds. The main use of fumaric acid is, however, as unsaturated acid component for the manufacturing of unsaturated polyester resins. Moreover, because of its double bond and two carboxylic groups, fumaric acid can be converted to several interesting derivates, comparable to succinic acid. An overview of relevant derivatives is given in Table 2-18.

Derivative	World production (t/year)	Route from fumaric acid to derivative	Main uses, drivers
Unsaturated polyester resins	13,000 t/a; established with fumaric acid from fossil resources	Polycondensation of phthalic anhydride in the presence of fumaric acid (or maleic anhydride, respectively)	Used almost exclusively as unsaturated acid components for the manufacturing of unsaturated polyester resins; Fumaric acid can replace maleic acid and maleic anhydride to produce polyesters with improved thermal stability and mechanical properties (greater hardness), but is more expensive and has a higher water content.
Tetrahydrofuran (THF)	1.4×10^5 t (1992)	Catalytic hydrogenation of fumaric acid	Competes with THF production from succinic acid
1,4-butanediol (BDO)	512,000 t/a (1995)	Catalytic hydrogenation of fumaric acid	Competes with BDO production from succinic acid
γ-butyrolactone (GBL)		Reductive amination of fumaric acid	Competes with GBL production from succinic acid
L-aspartic acid	13,000 t/a; established on industrial scale	Enzymatic amination of ammonium fumate by L-aspartate ammonia-lyase (aspartase)	Established industrial process, e.g. for the production of L-aspartic acid for the manufacture of the sweetener aspartame

Table 2-18: Routes from fumaric acid to derivatives

Derivative	World production (t/year)	Route from fumaric acid to derivative	Main uses, drivers
L-alanine	established on industrial scale	Fumaric acid is enzymatically converted to L-aspartic acid by immobilised aspartase, followed by decarboxylation of L-aspartic acid to L-alanine by immobilised *Pseudomonas dacunhae* cells, expressing L-aspartate-4-carboxy-lyase	Process established by Tanabe Seiyaku, can also be used for simultaneous production of aspartic acid and alanine.
Succinic acid	15,000 t/a	a) Side reaction of fumarase b) Fermentative production from fumaric acid as substrate	see Section 2.3.1

Table 2-18 continued: Routes from fumaric acid to derivatives

2.3.3 Aspartic acid

Production of aspartic acid

L-Aspartic acid can be manufactured by four different routes, with the enzymatic route being the preferred one for industrial L-aspartic acid production:

- Chemical synthesis via asymmetric amination of fumaric acid with ammonia
- Extraction from protein hydrolysates
- Fermentation, and
- Enzymatic amination of fumaric acid, catalysed by L-aspartate ammonia lyase (aspartase). Both immobilised enzymes or whole cell systems are employed in industrial scale processes.

L-Aspartic acid is produced in amounts of approx. 13.000 t/year, its main uses being the synthesis of the sweetener aspartame. For bulk applications, two strategies could be envisioned (see also Table 2-19):

- Cost reduction of fumaric acid, using the established enzymatic route for bulk aspartic acid production.
- Establishing a fermentative route for aspartic acid starting from carbohydrates. At present, fermentation routes are not cost-competitive with the enzymatic route.

Building block	World Production (million t/a)	Route from biomass to building block	Current status	Challenges	Main uses, market drivers
Aspartic acid	0.013	Enzymatic amination of fumaric acid, catalysed by L-aspartate ammonia lyase (aspartase)	Commercialised	- Reduce cost of the feedstock fumaric acid (see also Section succinic acid) - Increases in productivity for bulk applications; currently only satisfactory for specialty applications - Scale-up	Production of sweetener aspartame (10,000 t/a) and other specialties; Potential to make accessible analogs of high-volume chemicals such as 1,4-butanediol, tetrahydrofuran and butyrolactone (see also Section 2.3.1)
		Fermentation, starting from carbohydrates	Lab scale, presently not cost-competitive with enzymatic route	- Development of low-cost fermentation process - Metabolic engineering of production strain - Strive for high productivity, yield, and final titers - Lower cost fermentation substrates. - Low cost recovery process - Scale-up - System integration issues.	

Table 2-19: Key characteristics of the routes from biomass to the building block aspartic acid

Use of L-aspartic acid to derivatives

Availability of L-aspartic acid as a commodity would open up the opportunity to produce (Werpy, Petersen 2004, p. 31ff):

- *Amino-analogues of high-volume chemicals* such as 1,4-butanediol, tetrahydrofuran and butyrolactone (see also Section 2.3.1), targeting polymer and solvent applications. This requires the development of selective catalysts which allow the selective reduction of the carboxylic group in the presence of an amino group.
- *Anhydrides* by selective dehydration. This requires the development of appropriate catalysts.
- *Specialty polymers*, such as polyaspartic acid. The polymerisation should be analogous to the synthesis of polyglutamic acid which is a commercial process. Aspartic acid-based polymers could be substitutes for polyacrylic acid and polycarboxylates in applications such as detergents, water treatment, corrosion inhibition and super-absorbers.

2.3.4 1-butanol

Production of 1-butanol

1-butanol (n-butanol, butyl alcohol) is an aliphatic saturated C_4 alcohol. Production processes for 1-butanol with industrial importance are propylene hydroformylation (oxo synthesis), Reppe synthesis and crotonaldehyde hydrogenation, with propylene hydroformulation being the most important one. The annual world production of 1-butanol is in the order of magnitude of 2 million t/year.

1-butanol can be produced fermentatively by *Clostridium acetobutylicum* and related clostridia. The process is also known as acetone butanol ethanol (ABE) or solvent fermentation. In the first half of the 20th century, large-scale industrial processes were established in many countries for the fermentative production of acetone, butanol and ethanol from starchy substrates. The largest facility in the USA had an installed capacity of more than 18 million l. With respect to the production volume, ABE fermentation was the second-largest fermentative process after ethanol production (Section 2.1.1), but was abandoned until the 1980s because these chemicals could be made more cheaply from fossil oil sources (Dürre 1998; Gapes 2000; Girbal, Soucaille 1998; Nimcevic, Gapes 2000; Qureshi, Blaschek 2001a).

Research into the revitalisation of the process is ongoing, but is mainly restricted to laboratory experiments whereas only a very limited number of pilot scale processes are operated worldwide (Qureshi, Blaschek 2001a). The state of research in ABE fermentation can be characterised as follows:

Several clostridia, with the most extensively investigated one being *Clostridium acetobutylicum*, produce 1-butanol, acetone and ethanol from starch or glucose via several pathways which interact in a complex manner. During the acidogenic growth phase, organic acids such as lactic, acetic, butyric acid as well as H_2 and CO_2 are formed. In the stationary, solventogenic phase, acetone, 1-butanol and ethanol are formed and the previously formed acids are also metabolised. Most of the (iso-)enzymes involved have been characterised, and most of the corresponding genes have been cloned and sequenced. Elucidating the regulatory networks is the issue of ongoing research, as well as metabolic engineering approaches (Bennett 2005). Moreover, process engineering research is ongoing, with the aim of overcoming the following obstacles to cost-competitiveness with fossil-based processes:

- *Reduction of relatively high substrate costs*. On the one hand, cheap low-grade agricultural substrates which cannot be used for food or feed purposes, are favoured but only allow ABE fermentations in niche markets (Gapes 2000). On the other hand, lignocellulosic substrates are favoured. However, as *solventogenic clostridia* cannot hydrolyse cellulose, a hydrolytic pretreatment of the lignocellulosic substrates would be required (see also Section 2.5.1). But the whole genome sequence of *C. acetobutylicum* revealed inactive cellulase genes which might be activated by genetic modification for cellulose hydrolysis (Hüsing et al. 2003, p. 144).
- *Low yields, productivities and final concentrations*. Due to the inhibitory effects of both high glucose concentrations as well as high butanol concentrations, yields, productivities and final concentrations are usually too low for a commercially viable fermentation process (Table 2-20). Approaches to achieve higher productivities comprise the development of improved production strains by conventional mutagenesis, metabolically engineered production strains, employing fed-batch processes (Qureshi et al. 2004) and immobilised cells, and the continuous product removal to prevent product inhibition.
- *Downstream processing and product recovery*. The impact of recent process advances in ABE fermentation on production costs was assessed by Qureshi, Blaschek 2001a. The results are shown in Table 2-21. It shows that the largest cost reduction potentials lie in efficient and energy-saving product recovery techniques. As a consequence, there is a need to replace the usual and dominant distillation processes by other techniques (Vane 2005). Several online/in situ techniques of butanol removal have been tested, among them pervaporation, liquid-liquid extraction and gas stripping. The latter appeared to be most promising for cost-effective industrial applications (Ezeji et al. 2004). Absorption techniques have also been investigated (Qureshi et al. 2005).
- *Reliability, stability and reproducibility of the process*. The stability of ABE fermentation over time is not satisfactory: on the one hand, production strains are known to degenerate which is due to the localisation of several solventogenic genes on a megaplasmid which may get lost. It has been suggested to integrate all solventogenic genes in the bacterial chromosome or to stabilise the megaplasmid (Dürre 1998). On the other hand, substantial economic losses may be due to phage infection of the production process (Jones et al. 2000). Approaches for prevention of phage infection comprise the selection of phage-resistant productions strains as well

as sterile production processes (Jones et al. 2000). Moreover, so called "acid-crashes" are known in which the fermentation remains in the acetogenic stage and does not proceed to the solventogenic stage (Maddox et al. 2000).

Parameter	Typical fermentation with *Clostridium acetobutylicum*	Mutant *Clostridium beijerinckii* BA101
Final solvent concentration	20 g/l	27-29 g/l (33 g/l after supplementation with sodium acetate)
Ratio acetone:butanol:ethanol	3:6:1	3:16:1
Final butanol concentration	12 g/l	26 g/l (165 g/l with simultaneous pervaporation of butanol)
Type of fermentation	Batch or fed-batch	Fed-batch
Substrate	Glucose	Glucose, starch
Yield/fermentable sugars	29-33%	40-50%

Table 2-20: Typical performance parameters for ABE fermentations (Dürre 1998; Qureshi, Blaschek 2001a; Qureshi, Blaschek 2001b)

Process option	Product recovery	1-butanol production cost (US-$/kg)
Batch fermentation	Distillation	0.38-0.55
Batch fermentation	Pervaporation	0.14-0.39
Fed-batch fermentation	Pervaporation	0.12-0.37
Continous fermentation with immobilised cells	Pervaporation	0.11-0.36
Chemical synthesis from fossil feedstocks		1.21[19]

Table 2-21: Impact of different process options on the 1-butanol production costs (model calculations) (Qureshi, Blaschek 2001a)

Use of 1-butanol

The main use of 1-butanol is as a solvent and thinner for varnishes and lacqers, as well as applications as plasticizers (e.g. 1-butyl esters of phthalic, adipic, sebacic, oleic, azelaic, stearic, and phosphoric acids), butyl acetate, acrylic esters, butylamines, and glycol esters.

[19] According to experts' assessments, a shift from chemical synthesis to fermentative production of 1-butanol is only economically attractive, if the production cost of the bioroute falls below 0.44 US-$ (Qureshi, Blaschek 2001a).

2.3.5 1,4-butanediol

Production of 1,4-butanediol

The bifunctional alcohol 1,4-butanediol (BDO) is a versatile intermediate for the chemical industry. It is the most widely used of all the four-carbon-based diols in industry today. The worldwide capacity for 1,4-butanediol was approx. 512,000 t/a in 1995. 1,4-Butanediol is made on a large industrial scale by continuous hydrogenation of the 2-butyne-1,4-diol over modified nickel or palladium catalysts. Because of the increasing new market demand for polybutylene terephthalate (PBT) new production technologies were developed for 1,4-butanediol synthesis, among them (Haas et al. 2005):

- Acetoxylation of butadiene,
- Selective oxidation of butane to maleic anhydride, followed by hydrogenation,
- Hydroformulation of allyl alcohol,
- Epoxidation of butadiene.

A route from biomass has been described in Section 2.3.1: fermentative production of succinic acid from biomass, followed by catalytic reduction of succinic acid to 1,4-butanediol. DuPont's recent success with 1,3-PDO (Section 2.2.4) could well provide stimulus to develop a commercial bioroute to BDO in order to produce bio-based polybutylene terephthalate (PBT), but to the best of our knowledge, no economically viable process has been established yet.

Use of 1,4-butanediol

The bifunctional alcohol 1,4-butanediol is a versatile intermediate for the chemical industry. It reacts with dicarboxylic acids to yield polyesters, with diisocyanates to yield polyurethanes, and with phosgene to yield chloroformates. The main applications for butanediol are the production of cellular plastics, thermoplastic polyesters (e.g. polybutyleneterephthalate, PBT), hot-melt adhesives and plasticizers. Possible derivatives of 1,4-butanediol have been described in Section 2.3.5 and Table 2-16, among them

- bio-based polybutylene terephthalate (PBT). Petrochemically based PBT is already well established in the market: the demand in 1997 was 340,000 t, with a growth rate above 6% p.a. (Crank et al. 2005, p. 51; see also Table 2-16),
- bio-based polybutylene succinate (PBS),
- polyurethanes,
- γ-butyrolactone (GBL),
- tetrahydrofuran (THF), with further conversion to pyrrolidones or use as solvent,
- adipic acid, and
- pyrrolidones.

2.4 C_5 building blocks

2.4.1 Xylose, arabinose and xylitol, arabinitol

Production of xylose and arabinose

The pentoses xylose and arabinose are the main constituents of pentosans in hemicellulose. The economic viability of a biorefinery will also depend on the valorisation of pentosans from hemicelluloses.

Xylose and arabinose can be obtained from lignocellulosic biomass by combined thermomechanical treatment, acid hydrolysis, and eventually enzymatic treatment. A major challenge is the separation of these pentoses from other sugars present in lignocellulose hydrolysates in order to obtain a fairly clean feed stream of these sugars in a low-cost way (Werpy, Petersen 2004).

Use of xylose and arabinose

Major derivatives of xylose and arabinose are fermentation products (see also Section 2.5.1), furfural and its derivatives (see also Section 2.4.3), xylitol/arabinitol and their derivatives. The relevant routes bear much resemblance with routes from sorbitol to sorbitol derivatives (Section 2.5.2), and levulinic acid (see Section 2.4.2).

Building block	World Production (t/a)	Route from xylose to derivative; current status	Challenges	Main uses, market drivers
Furfural	200,000 to 300,000	Pentosan-containing biomass is hydrolysed to pentoses by dilute sulfuric acid, followed by cyclodehydration to furfural. Furfural is stripped from liquid phase by steam Established, used in large-scale commercial operations	Increases of the low yield due to polymerisation and degradation loss reactions (from presently 55% to 80% or higher); Avoiding of yield-loss side reactions and by-products (e.g. 5-methyl furfural, furyl methyl ketone, acetaldehyde, ethanol, methanol, acetic acid, formic acid); New catalysts; Reactor design; Improving product purity; Improve energy-efficiency; Improving mass transfer; Integration of furfural production with other biomass conversions (e.g. furfural production and fermentative use of cellulose hydrolysate)	Starting material for the production of derivatives listed in Table 2-26. Selective extractant in the refining of lubricating oils, diesel fuels, and vegetable oils for the separation of saturated and unsaturated hydrocarbons and of aromatic and olefinic compounds, respectively; Nematicide, fungicide; to replace other pesticides for environmental considerations see also Section 2.4.3
Fermentation products		see Section 2.5.1		
1,2,4 butanetriol		Fermentative conversion of xylose or arabinose, respectively by pathway engineered microorganisms; Lab stage	No natural strain known which fermentatively produces 1,2,4 butanetriol; Construction of synthetic pathways with genes from *Pseudomonas* and *E. coli* in *E. coli*; Strain and process development for pilot and large-scale production (Niu et al. 2003)	Direct use as industrial and military energetic material, less hazardous, but presently more expensive than nitroglycerin; direct use as propellant; Potential to substitute nitroglycerin if produced cheaper; Enantiopure D- and L-isomers are valuable chiral synthons, e. g. for synthesis of pharmaceutical drugs (http://www.frostchemlab.com/biosynthetic-pathways.htm)

Table 2-22: Key characteristics of the routes from xylose to its derivatives

Building block	World prod. (t/a)	Route from xylose to derivative; current status	Challenges	Main uses, market drivers
Sugar alcohols, xylitol, arabinitol		Catalytic hydrogenation of xylose/arabinose, analogous to sorbitol production from glucose (see Section 2.5.2)	Scale-up to large-scale operation Industrial implementation of a continuous process	Xylitol: non-caloric sweetener Starting material for further derivatizations (see below)
Xylaric, xylonic acid arabonic, arabinoic acid		Selective oxidation of xylitol or arabinitol	Yield increase (from 60% to > 90%); New catalysts which give higher yield; Simple oxidants (O_2, air, H_2O_2) at low concentrations; Tolerance to catalyst poisoning by constituents of bio-based feedstocks; Enzymatic oxidations without cofactors or effective cofactor regeneration	
Polyesters		Use of xylitol/arabinitol together with other glycols for production of unsaturated polyesters	Control of polymerisation/branching; Evaluation of resulting polyester properties; Development and scale-up of production processes for promising candidates	Use as copolymer in unsaturated polyester production; potential to provide polyesters with new properties
Ethylene glycol, propylene glycol		Hydrogenolysis of xylitol/arabinitol to glycols produced from renewable instead of fossil feedstocks.	Yield increase from now 80% to at least 90%; Development of efficient catalyst systems with specificity for C-C and C-O bonds and which are also tolerant to catalyst poisoning by components of the biomass sugar substrates; Low cost xylose feedstock economic assessment	Potential to produce large volume commodities from biomass instead of fossil resources. Use as an important building block for unsaturated polyesters. Use as deicer and automotive antifreeze component; Medium- to long-term goal
Levulinic acid	450 t/a	Acid treatment of pentosans and reduction step		see Section 2.4.2

Table 2-22 continued: Key characteristics of the routes from xylose to its derivatives

2.4.2 Levulinic acid

Production of levulinic acid

Levulinic acid (β-acetylpropionic acid, γ-ketovaleric acid, 4-oxopentanoic acid, $H_3C–CO–CH_2–CH_2–COOH$,) is the simplest γ-oxocarboxylic acid. Levulinic acid is a usual component of hemicellulose hydrolysates, which is present in the hydrolysate together with dissolved sugars and their degradation products, such as furfural, hydroxy-methylfurfural, acetic acid, formic acid, and methanol. These substances often act as inhibitory substances for fermentative conversions of the hydrolysates (e.g. Larsson et al. 1999).

Several routes have been described from biomass to levulinic acid:

- Industrially, levulinic acid is produced from polymeric carbohydrates such as cellulose or starch via the monomeric hexoses. The reaction is usually acid catalyzed: Enzymatic conversions of the polymers to hexoses (see Section 2.5) can also be employed in these processes. D-glucose is formed first and is then isomerized enzymatically to D-fructose (Section 2.5.1). D-Fructose is subsequently converted to hydroxymethylfurfural (Section 2.5.3), an intermediate that reacts further to form levulinic acid.
- The classical levulinic acid synthesis, the treatment of D-fructose with hydrochloric acid, is also being used.
- Levulinic acid can also be obtained in an analogous fashion from pentoses such as xylose if the acid treatment is followed by a reduction step.
- Levulinic acid is also accessible via ring cleavage of furfural (Section 2.4.2).
- Levulinic acid production has also been reported from petrochemical raw materials: It is obtained by ozonolysis of unsaturated hydrocarbons in a relatively sophisticated process.

This list of synthetic routes shows that in principle, levulinic acid could be made available from a broad range of carbohydrate sources. At present, levulinic acid has a status as an expensive and relatively small market specialty chemical, with a production of approx. 450 t/year and prices of 8.8 to 13.2 US-$/kg (Bozell et al. 2000).
Carbohydrates are usually converted to levulinic acids in a batch reactor by incubation with acid at elevated temperatures and pressures. Yields around 30% are obtained (Fang, Hanna 2002), which can be raised to 50-70% if improvements in the process design are applied (Bozell et al. 2000; Cha, Hanna 2002; Werpy, Petersen 2004, p. 47).

Building block	World Production (t/a)	Route from biomass to levulinic acid; current status	Challenges	Main uses, market drivers
Levulinic acid	450	Acid-catalysed dehydration of carbohydrates in batch reactors; Small scale industrial production	Processing cost reductions; Further increases of the yield (50-70%); Replacement of liquid catalysts by heterogeneous, solid acid catalysts; Improvement of catalysts, higher selectivity; Reactor and process design; Integration of levulinic acid production with other biomass conversions (e.g. levulinic acid production and fermentative use of cellulose hydrolysate)	Starting material for the production of derivatives listed in Table 2-24

Table 2-23: Key characteristics of the routes from biomass to levulinic acid

Use of levulinic acid

In principle, levulinic acid could be converted to numerous derivatives of industrial utility, provided it can be produced at low cost. Levulinic acid reacts both as a ketone and as a carboxylic acid. Table 2-24 gives an overview of possible levulinic acid derivatives.

Derivative	Route from levulinic acid to derivative	Main uses, drivers
Methyl tetrahydrofuran (MTHF)	Reduction and dehydration	Similar chemical properties as tetrahydrofuran; Used as a specialty solvent; Used as reactant for production of chemicals, e.g., 2-methylpyrrolidine and N-substituted 2-methylpyrrolidines; Could be used as fuel oxygenates; drivers: environmental legislation, costs
Levulinate esters	Esterification	Could be used as fuel oxygenates; drivers: environmental legislation, costs
Angelica lactone	Elimination of water on prolonged heating of levulinic acid	Intermediate
γ-Valero-lactone	Catalytic hydrogenation of levulinic acid to lactones	Solvents; use for synthesis of analogues of N-methyl pyrrolidones
5-Methyl-2-pyrrolidone	Reductive amination	Solvents, use for synthesis of analogues of N-methyl pyrrolidones

Table 2-24: Derivatives of levulinic acid

Derivative	Route from levulinic acid to derivative	Main uses, drivers
δ-Amino-levulinic acid	Several routes possible	Broad-spectrum biodegradable herbicide; none of the proposed synthetic routes suitable for large-scale manufacture due to multistep syntheses, expensive reagents, toxic intermediates
Diphenolic Acid	Reaction of levulinic acid with phenol	Potential to replace Bisphenol A in polycarbonate production if cost-competitive
1,4-pentanediol	Hydrogenation	Use as bio-based diol in polyesters
Succinic acid	Oxidation	see Section 2.3.1
Acrylic acid	Oxidation	see Section 2.2.5
β-Acetyl-acrylic acid		Use in copolymerisation with other monomers for enhancement of polymer properties

Table 2-24 continued: Derivatives of levulinic acid

Although levulinic acid allows the synthesis of a large family of industrially relevant derivatives, this is mainly in the lab stage, and it remains to be assessed whether this potential can be realised on a larger scale. This requires the optimisation of levulinic acid production itself (higher yield, higher selectivity in dehydration of carbohydrates, lower production costs), as well as research into potential derivatives.

2.4.3 Furfural

Production of furfural

Furfural (2-furancarbonal, 2-furaldehyde, furfuraldehyde, $C_5H_4O_2$), is a chemical of fundamental importance as it is the starting material for the industrial production of almost all furan compounds. It is produced from biomass in amounts of 200,000 to 300,000 t/a worldwide. Feedstock for furfural production is (waste) biomass rich in pentosan, e.g. corn cobs, oat hulls, almond husks, cottonseed hull bran, birch wood, bagasse, sunflower husks. They all have a pentosan content between 25-30% (dry substance) and are therefore potential raw materials.

For the industrial production of furfural, the raw material containing pentosan is treated with aqueous acid at elevated temperature (steam injection). Pentosan is hydrolyzed to pentoses, which are dehydrated to furfural. Furfural is usually recovered from the liquid phase by steam stripping. Due to undesired loss reactions, especially degradation reactions of pentoses and furfural, and polymerisation reactions, the present industrial furfural reactors have a yield in the order of only 55%. Among the undesired by-products are the isomers 5-methyl furfural (concentrations ranging from 0.3 to 0.9%) and 2-furyl methyl ketone (0.05 to 0.35%), as well as several alcohols, organic acids and aldehydes. Removal of these high-boiling impurities is possible by distillation, but is usually considered too expensive, thereby impairing the purity of the furfural product.

In order to expand the use of furfural further beyond its established uses, optimisation of the furfural production process is necessary. Several process design improvements have been developed to pilot scale in recent years which lead to higher yields (up to 80%) due to reduced side reactions and improved product recovery (Cha, Hanna 2002). Additional R&D needs are listed in Table 2-25.

Building block	World Production (t/a)	Route from biomass to furfural; current status	Challenges	Main uses, market drivers
Furfural	200,000 to 300,000	Pentosan-containing biomass is hydrolysed to pentoses by dilute sulfuric acid, followed by cyclodehydration to furfural. Furfural is stripped from liquid phase by steam. Established, used in large-scale commercial operations	Increases of the low yield due to polymerisation and degradation loss reactions (from presently 55% to 80% or higher); Avoiding of yield-loss side reactions and by-products (e.g. 5-methyl furfural, furyl methyl ketone, acetaldehyde, ethanol, methanol, acetic acid, formic acid); New catalysts; Reactor design; Improving product purity; Improve energy-efficiency; Improving mass transfer; Integration of furfural production with other biomass conversions (e.g. furfural production and fermentative use of cellulose hydrolysate)	Starting material for the production of derivatives listed in Table 2-26. Selective extractant in the refining of lubricating oils, diesel fuels, and vegetable oils for the separation of saturated and unsaturated hydrocarbons and of aromatic and olefinic compounds, respectively. Nematicide, fungicide; to replace other pesticides for environmental considerations

Table 2-25: Key characteristics of the routes from biomass to furfural

Use of furfural

In addition to the direct uses of furfural as extractant and pesticide (Table 2-25), it is of great importance as starting material for the industrial production of almost all furan compounds. The chemistry of converting furfural to its derivatives is well developed and provides many versatile industrial chemicals by simple straightforward operations. An overview of established furfural derivatives is given in Table 2-26.

Derivative	World production (t/year)	Route from furfural to derivative	Main uses, drivers
Furfuryl alcohol	Capacity 120,000 to 180,000 (60% of furfural) Consumption 106,500 in 1998	Hydrogenation of furfural	Main uses are: Acid-catalyzed resinification for various different resins (> 75,000 t/a); Solvent; Production of other chemicals. Actual worldwide production capacity exceeds consumption by 30% so that the furfuryl alcohol plants are run on demand. Price wars are common. Consumption is concentrated in the industrialized countries where demand resides primarily in the foundry industry.
Tetrahydro-furfuryl alcohol		Vapor-phase hydrogenation of furfuryl alcohol with a nickel catalyst	Specialty solvent for dyes, resins, lacquers in commercial and industrial cleaners mainly employed in the automotive and equipment industries, intermediate in pharmaceuticals and fine chemicals synthesis
Furfuryl-amine		Reductive amination of furfural	Pharmaceutical synthesis (diuretic Furosemide)
Furoic acid		Oxidation of furfural	
Furan-acrylic acid		Perkin reaction	
Furylidene ketones		Aldol condensations	
Tetrahydrofuran (THF)	$1.4x10^5$t (1992)	Hydrogenation	Provides already today a biomass-based alternative to THF synthesis via dehydration of 1,4-butanediol THF could in future also become available via succinic acid or fumaric acid (see Sections 2.3.1 and 2.3.2)
Levulinic acid (4-oxovaleric acid)	450 t/a	Ring-cleavage	see Section 2.4.2
Maleic anhydride		Ring-cleavage	Alternative to maleic anhydride production by catalytic oxidation of benzene or oxidation of C_4 hydrocarbons
Resins	> 75,000 t/a	Acid-catalyzed resinification: Condensations of furfural, furfurylalcohol or tetrahydrofurfurylalcohol with formaldehyde, phenol, acetone, or urea	Many different applications which make use of the excellent thermosetting properties, most notably high corrosion resistance, low fire hazard and extreme physical strength of these resins main use in foundry industry as binders to produce sand cores and molds for metal castings

Table 2-26: Derivatives of furfural

Neither the production of furfural nor its derivatisation includes biotechnical processes, so that in a strict sense, furfural does not comply with the definition chosen in the BREW project. Furfural was nevertheless included because of its bulk production from

biomass already today, its diverse and versatile derivatives, and its importance in integrated concepts which aim at valorising all constituents of biomass.

2.5 C_6 building blocks

2.5.1 Sucrose and Glucose

At present, low molecular weight carbohydrates are preferable as raw materials for basic organic chemicals because organic commodity chemicals, also of low molecular weight, can be more expediently obtained from them than from polysaccharides. At present, glucose obtained from starch is the preferred feedstock. In contrast, fructose has a lower potential because of its much higher price and its more capricious and less developed basic chemistry (Lichtenthaler, Peters 2004).

Production of sucrose and glucose

D-Glucose (D-glucopyranose), $C_6H_{12}O_6$, is a six-carbon sugar (hexose) and by far the most abundant monosaccharide. Most glucose is bound up in the long-chain polymers starch and cellulose which are composed of anhydroglucopyranose units connected through α- and β-linkages, respectively. Therefore, manufacturing processes are required to release glucose from these polymers. Sucrose is a nonreducing disaccharide, composed of glucose and fructose.

Table 2-27 provides an overview of the key characteristics of the synthetic routes from biomass to the building blocks sucrose and glucose.

Production of sucrose

Main sources for sucrose are sugar cane and sugar beet from which sucrose is extracted in a technical process. This is an established and ripe technology. Potentials for improvement lie in the valorisation of by-products, in the reduction of energy and process aids demand of the production process, and in system integration issues. Worldwide production of raw sugar is around 125 to 130 million/year, with a share of sugar cane of 67-70% (data from 1990-1992). Together with starch-derived glucose, sucrose (in the form of molasses) is the major carbohydrate feedstock of low molecular weight for the production of chemicals.

Production of glucose from starch

Glucose-containing syrups can be obtained from the hydrolysis of starch or cellulose. However, the only raw material used for commercial production of glucose-containing syrups today is starch. The global starch production was 48.5×10^6 t in 2000. In worldwide perspective, the main starch sources are maize, manioc/cassava, wheat and potatoes, with 39.4×10^6 t (81%) maize starch, 4.1×10^6 t (8%) wheat starch, 2.6×10^6 t (5%) potato starch and 2.5×10^6 t (5%) tapioca starch and others (LMC International 2002). Other starch sources are only of minor or local relevance, e.g. amaranth, arrowroot, banana, canna, cow cockle, faba/mung beans, kouzou, lentils, lotus roots, quinoa, sago palm, sorghum, sweet potatoes, taro, water chestnut, wild rice, and yam. Starch is predominantly produced in highly industrialized countries such as the United States, the EU and Japan.

State of the art of industrial glucose syrup processing from starch are enzymatic hydrolysis processes. Hydrolysis of starch by acids or combined acid/enzymatic hydrolysis processes are also employed. Usually, enzymatic hydrolysis is carried out with immobilised α- or β-amylases, glucamylase, pullulanase and xylanases. The different substrates and reactions specificities of these enzymes allow the tailoring of saccharide distributions in the hydrolysate.

The application of tools of screening for new enzyme activities and for the engineering of enzyme properties in recent years has led to a considerable improvement in the availability and scope of starch-processing enzymes, and in improvements of their performance, e.g. by adapting their pH optimum, their thermostability, reaction and substrate specificities, and efficacy (Crabb, Mitchinson 1997; Crabb, Shetty 1999; Nigam, Singh 1995), thus allowing the starch processor to tailor the degree of hydrolysis and the saccharide range and distribution accordingly.

Production of glucose from lignocellulose

A major challenge is to use not only sucrose and starch for the manufacturing of glucose syrups, but also cellulose (Himmel et al. 1999; Lynd et al. 2002). Cellulose is a β-1,4-polyacetal of glucose and one of the main cell wall constituents of all major plants where it forms complexes with hemicellulose and lignin. The annual yield of cellulosic matter resulting from photosynthesis amounts to approximately 1.3×10^9 tons. In order to bring cellulose into a form that is amenable to biotechnological valorisation, a combination of thermo-mechanical treatment (e.g. steam explosion), acid hydrolysis and enzymatic hydrolysis is favoured. In the USA, major research contracts deal with the optimisation of the cellulase hydrolysis (NREL/DOE in co-operation with the leading enzyme companies Novozymes and Genencor), with the aim of producing ethanol from lignocellulosic feedstocks. The aim is to achieve an at least 10-fold reduction in cost of enzymes for lignocellulosic biomass conversion. This goal can only be achieved if both the enzyme production costs are decreased and also the cellulase performance is improved. Approaches to reduce the enzyme production costs comprise reduced

feedstock costs, reduced enzyme recovery costs, on-site production, strain enhancement and increased fermentation yield. Both simultaneous saccharification and fermentation processes where cellulose hydrolysis and ethanol fermentation take place simultaneously in one tank and two-stage processes are being evaluated.

In order to increase cellulase activity, enzymes with improved thermostability and higher specific activities are tested. In 2004, Genencor and Novozymes reported that they were successful in reaching the 10-fold cost decrease target.[20] According to NREL model calculations, their cellulases could be produced at 0.20-0.50 US-$/gallon ethanol which is more than 10 times lower than existing commercial cellulases. These results from model calculations must still be validated at pilot scale in order to test whether cellulase costs can in practice be lowered to 0.10 US-$/gallon ethanol in order to bring ethanol production costs into acceptable ranges.

Additional challenges are posed by the detoxification of cellulosic hydrolysates from constituents such as weak acids, furan derivatives and phenolic substances which could act as inhibitors for subsequent biotechnological valorisation. For detoxification, treatment with laccases, chemical precipitation and extraction or ion exchange are being considered. Moreover, production strains with high tolerance towards these inhibitors and process design options (e.g. fed-batch) are being tested (Luo et al. 2001; Palmqvist et al. 2000b; Palmqvist et al. 2000a; Himmel et al. 1999). Another challenge is to develop solutions for the complete conversion of all sugars (hexoses and pentoses; see also C_5 building blocks, Section 2.4).

A long-term goal is the genetic modification of the lignocellulosic feedstock biomass itself to make its hydrolysis to fermentable sugars easier (Boudet et al. 2003; Pilate et al. 2002; Reddy, Yang 2005; Section 2.7.8).

[20] Genencor Press Release of October 21, 2004 (http://www.genencor.com/wt/gcor/ pr_1098313606); Novozymes Press Release of April 26, 2004 (http://www.novozymes.com /cgi-bin/bvisapi.dll/ press/press.jsp?id=28895&lang=en)

Building block	World Production (million t/a)	Route from biomass to building block	Current status	Challenges	Main uses, market drivers
Sucrose	125 to 130, (data from 1990-1992)	Extraction from sugar cane (share of total production: 67-70%) and sugar beet (share of total production: 30-33%)	Established, technically mature, used in large-scale commercial operations	- Valorisation of by-products, - Reduction of energy and process aids demand of the production process - System integration issues	- Sweetener in food and beverages - Used as feedstock for fermentations and as feedstock for (bio)chemical non-food valorisation, but potential still underexploited - Glucose is transformed to sorbitol by hydrogenation. Sorbitol is used notably as an intermediate for surfactants, PEP for PU.
Glucose	5 to 20	a) Enzymatic hydrolysis of starch	Established, technically mature, used in large-scale commercial operations	- Further, incremental improvement of scope, production costs and performance of enzymes	
		b) Hydrolysis of cellulose through combined thermomechanical treatment, acid hydrolysis, cellulase hydrolysis	Pilot scale	- Enzyme production costs must be lowered - Detoxification of inhibitory substances in the cellulose hydrolysate - Valorisation of all constituents of the cellulose hydrolysate (hexoses and pentoses)	- Potential as abundantly available, cheap feedstock for fermentations and as feedstock for (bio)chemical non-food valorisation - Driver: Bioethanol production from lignocellulosic biomass

Table 2-27: Key characteristics of the routes from biomass to the building blocks sucrose and glucose

Use of C_6 building blocks to their derivatives

Use of glucose

Major glucose derivatives that are produced commercially on a large scale are fructose, sorbitol and alkylpolyglycosides (non-ionic surfactants) (Table 2-28). Moreover, glucose (as well as sucrose, starch, pentoses, glycerol, and also fatty acids and proteins) can be used as substrates for fermentation products. An overview of relevant fermentation products derived from glucose or sucrose is given in Table 2-29, with ethanol, L-glutamic acid, citric acid, L-lysine, gluconic acid as well as antibiotics and industrial enzymes being quantitatively the most important. Some of these products are considered valuable building blocks and are described in more detail in other chapters. In the past, ABE fermentation for the production of acetone and 1-butanol was also carried out on large industrial scale, being the second largest fermentation process after ethanol in terms of annual production volume. The last large-scale commercial ABE fermentation was, however, abandoned in 1982.

Moreover, major entry reactions for the derivatization of D-glucose have been established, among them

- Mercaptalisation to the acyclic dithio acetals,
- Isopropylidenation to furanoid systems,
- Generation of pyranoid structures, such as glucosides, glucals, and hydroxyglucalesters,
- Conversion to furanic building blocks,
- Conversion to cyclo-pentaoid products, such as kojic acid (Lichtenthaler, Peters 2004).

However, they are at present not of economic importance for bulk chemicals. Therefore, the chemical potential of glucose is largely untapped and not yet exploited systematically, mainly because equivalent products based on petrochemical raw materials are still cheaper (Lichtenthaler, Peters 2004).

Derivative	World Production (million t/a)	Route from glucose to derivative	Current status	Challenges	Main uses, market drivers
Fructose	Glucose–fructose syrups: 10.1 (dry basis, 1995) Crystalline fructose: 0.24	Enzymatic or acid hydrolysis of starch to glucose syrups, followed by enzymatic isomerization of glucose to fructose with glucose isomerase	Established, technically mature, used in large-scale commercial opera-tions. Competes with alternative routes from alternative feedstocks: - enzymatic hydrolysis of inulin, - acid hydrolysis of sucrose to glucose and fructose, chromatographic separation of glucose and fructose - enzymatic sucrose hydrolysis by invertase (b-d-fructofuranosidase) from *Saccharomyces cerevisiae*	Genetically modified enzymes in order to directly obtain fructose purity of 90% in the isomerization step; Crystallisation of fructose from lower purity high-fructose syrups; Single unit operation for enzymatic isomerisation and glucose/fructose separation.	Main uses as sweetener in food and beverages drivers: only moderate potential for non-food valorisation due to relatively high price and rather capricious and less developed basic chemistry than e.g. glucose, sorbitol drivers: can be converted to levulinic acid and 5-hydroxymethylfurfural (see Section 2.4.2 and Section 2.5.3)
Sorbitol D-glucitol	1.1	a) Hydrogenation of glucose with nickel catalysts in batch processes	Established, technically mature, used in large-scale commercial operations	Few. Implementation on industrial scale Continuous process	Main uses in food, as non-caloric sweetener, moisture conditioner; competes with glycerol. Drivers: commercialisation of non-food derivatives, see Section 2.5.2
		b) Fermentative production of sorbitol and gluconic acid from fructose and glucose by *Zymomonas mobilis*	Laboratory stage, of academic interest	cf. Silveira, Jonas 2002	unlikely to become competitive with hydrogenation of glucose (a)

Table 2-28: Key characteristics of the routes from glucose to its derivatives

Derivative	World production (million t/a)	Route from glucose to derivative	Current status	Challenges	Main uses, market drivers
Alkylpoly-glycosides (APG)	0.05-0.07	a) Acid-induced glycosidation of glucose with a long chain fat alcohol b) Transglycosylation of a short-chain alkyl glucoside with long-chain alkanol	Established, used in large-scale commercial operations	Cost reduction	Use as surfactants, detergents, personal care; Drivers: environmental considerations, can be manufactured from renewable raw materials only, are biodegradable, non-toxic, low skin irritation
Methyl-∀-D-glucoside		Heating glucose and methanol in the presence of anhydrous hydrogen chloride	Commercial, industrial small scale production		Insulating foams
5-hydroxy-methylfurfural		Dehydration of fructose			Phenolic and urea – formaldehyde-based plastics see Section 2.5.3

Table 2-28 continued: Key characteristics of the routes from glucose to its derivatives

Building block	World Production (million t/a)	Route from biomass to building block	Current status, challenges	Main uses, market drivers, remarks
Ethanol	32	a) Fermentation of sucrose or starch to ethanol (95%) b) Chemical synthesis (5%)	Commercialised from sucrose and starch feedstocks, small pilot scale from lignocellulosic feedstocks	see Section 2.1.1
Acetone	3	ABE fermentation with *Clostridium acetobutylicum*; other products 1-butanol, ethanol	abandoned in 1982	see Section 2.3.4
L-glutamic Acid	1.5	Fermentation	commercialised	
1-butanol	1.2	ABE-fermentation	historical, abandoned in 1982	see Section 2.3.4
Citric Acid	1.0	Fermentation	commercialised	

Table 2-29: Commercialised products derived from glucose, sucrose or starch by fermentation or enzymatic conversion

Building block	World prod. (million t/a)	Route from biomass to building block	Current status, challenges	Main uses, market drivers, remarks
Glycerol	0.75	a) Synthetic glycerol from propylene (10%) b) Natural glycerol as byproduct of the (enzymatic) conversion of fats and oils to fatty acids or fatty acid methyl esters (90%) c) Fermentation d) Co-product of bio-diesel production (fatty acid methyl esters)	a) commercialised b) commercialised c) developed to commercial scale, but industrially not important	see Section 2.2.2
L-Lysine	0.7	Fermentation with *Corynebacterium* or *Brevibacterium*		
Acetic acid	a) 7 b) 0.19	a) Carbonylation of methanol b) Fermentation for food purposes	b) commercialised only for food purposes	see Section 2.1.2
Lactic acid	0.15	a) Reaction of acetaldehyde with hydrogen cyanide followed by the hydrolysis of the resultant lactonitrile b) Fermentation	a) and b) commercialised, b) more important than a)	see Section 2.2.1
Propionic acid	0.13	a) Chemical synthesis via carbonylation of ethylene, oxidation of propanal, or direct oxidation of hydrocarbons b) Fermentation with *Propionibacterium shermanii*	b) commercialised, but confined to small-scale specific purposes (food, fragrances)	
Gluconic acid	0.1	Chemical, electrolytic, catalytic, or biochemical oxidation of glucose or glucose-containing raw materials; mainly fermentative glucose oxidation by *Aspergillus* or *Gluconobacter*	commercialised	Gluconic acid and sodium gluconate are used as complexing agents for detergents. They can replace aminocarboxylic salts (like EDTA) in some formulations
Vitamin C	0.08	a) Reichstein process (six chemical steps plus 1 fermentative oxidation step (D-sorbitol to L-sorbose) b) Bacterial biotransformations for the synthesis of Reichstein intermediates (production of 2-keto-L-gulonate by oxidation of D-glucose or D-sorbitol or L-sorbose) c) Bioconversion of 2-keto-L-gulonate to L-ascorbic acid d) Direct biosynthesis of L-ascorbic acid in eucaryotes (plants, algae, yeast)	b) is gaining importance over a) c) and d) are industrially not relevant	
L-Sorbose	0.05	Fermentation	commercialised	
Antibiotics		Fermentation, enzymatic conversion		

Table 2-29 continued: Commercialised products derived from glucose, sucrose or starch by fermentation or enzymatic conversion

Building block	World Production (million t/a)	Route from biomass to building block	Current status, challenges	Main uses, market drivers, remarks
Industrial enzymes		a) Fermentation, also heterologous expression in GMOs b) Transgenic plants	a) commercialised b) mainly lab to pilot stage	
Xanthan	0.04	Fermentation with *Xanthomonas campestris*	commercialised	Food, pharma, personal care, oil drilling
Sugar alcohols, e.g. erithritol	0.03		commercialised	
L-Threonine	0.03	Fermentation	commercialised	
Vitamin B2	0.03			
Malic Acid	0.025	a) Hydration of maleic anhydride b) Enzymatic conversion of fumaric acid to L-malic acid	a), b) commercialised	
Succinic acid	0.015	a) Ring-opening oxidation of cyclic compounds b) Fermentation, also by GMOs	a) commercialised b) pilot stage to commercialisation	see Section 2.3.1
L-Aspartic acid	0.013	Enzymatic amination of fumaric acid by aspartase	commercialised	see Section 2.3.3
Fumaric acid	0.012	Fermentation, enzymatic conversion	commercialised	see Section 2.3.2
L-Phenylalanine	0.01		commercialised	
Pullulan	0.01	Fermentation with *Aureobasidium*	commercialised	Packaging
Cyclodextrins	0.005	Enzymatic degradation of starch with cyclodextrin glycosyltransferase	commercialised	
Itaconic acid	0.004	Fermentation with *Aspergillus terreus*	commercialised	

Table 2-29 continued: Commercialised products derived from glucose, sucrose or starch by fermentation or enzymatic conversion

Building block	Annual World Production (million t/a)	Route from biomass to building block	Current status, challenges	Main uses, market drivers, remarks
L-Arginine	0.0015		commercialised	
L-Alanine	0.0012		commercialised	
L-Trypthophane	0.0012		commercialised	
L-Glutamine	0.0010		commercialised	
L-Hydroxyproline	0.0001		commercialised	
L-Leucine	0.0008		commercialised	
L-Proline	0.0008		commercialised	
L-Serine	0.0003		commercialised	
L-Histidine	0.0003		commercialised	
L-Isoleucine	0.00055		commercialised	
L-Valine	0.00005		commercialised	
Hyaluronic acid	0.00005	Fermentation with streptococci	commercialised	Fine chemical for pharmaceutical applications
Bacterial cellulose		Fermentation with *Acetobacter xylinum*	commercialised	Fine chemical for pharmaceutical applications
Gellan		Fermentation by *Sphingomonas paucimobilis*	commercialised	
Poly-(-glutamic acid		a) Chemical synthesis b) Fermentation	b) commercialised	
Poly-,-lysine		a) Chemical synthesis b) Fermentation	b) commercialised	
Vitamin A		Fermentation	commercialised	
Vitamin B1		Fermentation	commercialised	
Vitamin B12	0.000020	Fermentation	commercialised	
Biotin		Fermentation	commercialised	
Folic acid		Fermentation	commercialised	
Pantothenic acid		Fermentation	commercialised	
Kojic acid		Fermentation with *Aspergillus oryzae*	commercialised	

Table 2-29 continued: Commercialised products derived from glucose, sucrose or starch by fermentation or enzymatic conversion

Building block	Annual World Production (million t/a)	Route from biomass to building block	Current status, challenges	Main uses, market drivers, remarks
1,2-Propanediol	1.5	a) Synthetised from propylene oxide and water b) Catalytic reduction of fermentatively produced lactic acid c) Fermentation with pathway-engineered GMO of hexoses and pentoses	a) commercialised b, c) lab stage	see Section 2.2.1
1,3-Propanediol	>0.08	a) Catalytic conversion of either ethylene oxide, acrolein or glycerol b) Bacterial fermentation of glycerol c) Mixed culture fermentation or two-stage fermentation of glucose d) Fermentation with pathway-engineered *E. coli* from glucose	a) commercialised, b, c) lab stage d) pilot scale, to be commercialised	see Section 2.2.4
2-propanol (isopropanol, isopropyl alcohol)		Modified ABE fermentation with *Clostridium*		

Table 2-30: Products derived from glucose, sucrose or starch by fermentation or enzymatic conversion on large pilot scale or lab stage, or unknown status

Building block	Annual World Production (million t/a)	Route from biomass to building block	Current status, challenges	Main uses, market drivers, remarks
3-Hydroxypropionic acid		a) Synthetised from acrolein b) Fermentation by pathway engineered microorganisms	a) commercialised b) lab stage	see Section 2.2.3
Glyoxylic acid		a) Oxidation of glyoxal with 65% nitric acid; main byproduct is oxalic acid b) Fermentation		
Oxalic acid	0.124 (1990)	a) Oxidation of carbohydrates/molasses/agricultural waste with nitric acid b) Oxidation of ethylene glycol with nitric acid c) Oxidation of propylene with nitric acid d) Production from carbon monoxide e) Fermentative production from carbohydrates or lipids with fungi such as Aspergillus	a-d) commercialised, with production volumes a) > c) > b, d) e) lab – pilot stage	synthetic intermediate, reducing agent, precipitant for calcium ions, complexing agent for the salts of heavy metals
Butyric Acid	0.05	a) Liquid-phase oxidation of n-butyraldehyde with oxygen b) Fermentation with *Clostridium butyricum* or *Bacillus butylicus*	a) commercialised b) lab stage	
2,3-butanediol		a) Synthesis from butenes from crack gases b) Fermentation	a) commercialised b) abandoned	
1,2,4-butanetriol		a) $NaBH_4$ reduction of esterified D,L malic acid b) Fermentation with pathway engineered *E. coli* from xylose or arabinose	a) commercialised b) lab stage	see Section 2.4.1
cis-cis-muconic acid		Fermentative production by pathway engineered *E. coli*	lab stage	

Table 2-30 continued: Products derived from glucose, sucrose or starch by fermentation or enzymatic conversion on large pilot scale or lab stage, or unknown status

Building block	Annual World prod. (million t/a)	Route from biomass to building block	Current status, challenges	Main uses, market drivers, remarks
Alginate	0.03	a) Isolation from brown algae biomass b) Fermentative production by *Azotobacter/Pseudomonas*	a) commercialised b) lab stage	
Curdlan		Fermentation by *Agrobacterium* and *Rhizobium*		Food, fine chemical
Chondroitin				Fine chemical for pharmaceutical and analytical research applications
Heparin				Fine chemical for pharmaceutical and analytical research applications
Cyanophycin		Heterologous production of this cyanobacterial polymer in bacteria	lab stage	
Polyhydroxyalkanoates	0.001 (cumulative)	a) Bacterial fermentation b) in transgenic plants	lab to pilot scale	Packaging
Scleroglucan		Fermentation with *Sclerotium* or *Schizophyllum*		Fine chemical for pharmaceutical applications
Sphingan		Fermentation by *Sphingomonas paucimobilis*		
Indigo	0.03	a) Chemical synthesis: ring closure of N-phenylglycine with sodium amide b) Fermentation of glucose using recom-binant *Escherichia coli*	a) established at large industrial scale b) lab to pilot scale, never commercialised	

Table 2-30 continued: Products derived from glucose, sucrose or starch by fermentation or enzymatic conversion on large pilot scale or lab stage, or unknown status

Use of sucrose

Sucrose, produced in amounts of 130 million t/year, is used for
- direct use as sweetener in food and beverages,
- as substrate for fermentations (see Table 2-29 and Table 2-30).

Valorisation of sucrose for non-food purposes is hampered by the difficulty of carrying out regioselective chemical reactions at a single hydroxylgroup without protection of the other seven hydroxyl groups. Derivatives of industrial relevance or potential non-food applications are the following (Lichtenthaler, Peters 2004):

- *Isomaltulose and derivatives*. Catalysed by immobilized glucosyltransferase from *Protaminobacter rubrum*, sucrose is converted to its isomer isomaltulose at a volume of 60,000 t/a. Isomaltulose can be converted further by the following reactions:
  - Hydrogenation to isomalt, a low-caloric sweetener,
  - Reductive amination to isomaltamine, which can be further reacted with fatty acid halides to non-ionic, biodegradable detergents, or with methacrylic acid to polymerisable acrylamido-disaccharides.
  - Oxidation to glucosyl-arabinonic acid or its lactone,
  - Acidic dehydration to 5-(α-D-glucosyloxymethyl)-furfural (α-GMF), which could give rise to polymerisable derivatives with double bonds after aldol-type condensations, leading to novel hydrophilic polymers. Oxidation of α-GMF and subsequent esterification with long-chain alcohols could give a new type of non-ionic surfactants or materials with favourable liquid crystalline properties. These product types could also be accessible via reductive amination of α-GMF and subsequent N-acylation with fatty acids.
- *Sucrose ethers*. Etherification of sucrose with long-chain epoxides gives potential non-ionic surfactants or liquid crystal materials. If sucrose is etherified with propylene oxide, it can be used as a replacement of fossil-derived di- and polyols in polyurethan synthesis.
- *Oxidation of sucrose*. *Agrobacterium tumefaciens* dehydrogenase regiospecifically oxidises sucrose to 3g-ketosucrose, making possible specific modifications of this carbonyl function.
- *Sucrose esters*. Esterification of sucrose yields food and cosmetic emulsifiers and surfactants. The octa-fatty acid ester of sucrose (Olestra, Olean) has been approved as a dietary fat substitute.

2.5.2 Sorbitol

Production of sorbitol

Sorbitol (D-glucitol, D-sorbitol, D-glucohexane-1,2,3,4,5,6-hexaol) is produced on large industrial scale (production 1.1 million t/year) by catalytic hydrogenation of glucose in a batch process. For conversion of biomass to glucose see Section 2.5.1. A fermentative process has been suggested in which *Zymomonas mobilis* converts fructose and glucose to sorbitol and gluconic acid (Silveira, Jonas 2002). It is, however, unlikely that this fermentative process can replace the simple and technically mature catalytic hydrogenation process (see also Table 2-28). Further development of the catalytic hydrogenation process could be the industrial implementation of a continuous process, replacing the present batch processes. Sorbitol is used in food, as a sweetening agent, as a stabilizer of humidity, and raw material for other products (e.g. vitamin C, surfactants, polyurethanes).

Use of sorbitol

Derivatives of industrial relevance or potential non-food applications of sorbitol are the following:

- *Ascorbic acid, vitamin C*. Sorbitol is converted via sorbose or 2-ketogulonic acid in combined biotechnological and chemical processes to vitamin C (Hancock, Viola 2001; Hancock, Viola 2002). The world production volume is approximately 80,000 t/year.
- *1,4-Sorbitan*. Sorbitol is dehydrated to sorbitan, which is subsequently esterified with fatty acids. Such sorbitan esters are commercially produced at approximately 50,000 t/year and are used as non-ionic surfactants and as solubilizers and emulsifiers, e.g. in cosmetics.
- *Polyetherpolyols*. Sorbitol can be polymerised to polyetherpolyols which can be used as intermediates for the synthesis of polyurethanes.
- *Isosorbide*. Selective dehydration of sorbitol gives the anhydrosugar isosorbide. Presently, it is produced commercially at rather low volumes of 800 t/year for the synthesis of isosorbide dinitrate, used in pharmaceuticals as a vasodilatator, and of dimethylisosorbide which is used as a solvent today in cosmetics. Dimethylisosorbide could be used in the future in many other (industrial) applications.

  Isosorbide bears the potential to (partially) replace fossil-derived ethylene glycol in polymers such as PET by a "green" diol. Isosorbide was shown to confer a higher glass transition temperature to polyethylene isosorbide modified terephthalate (PEIT), which is thought to be a favourable property e.g. for use in hot-fill containers. Additional applications in unsaturated and saturated polyesters and

polyurethans are being tested. High purity Isosorbide is required for polymer applications. The ROQUETTE Company (France) has developed and is commercializing a special grade of high purity isosorbide dedicated to these polymers markets.

Isosorbide diesters are presently under evaluation for their potential use as new speciality plasticizers. They could serve e.g. as non-toxic replacements of some phthalates based plasticizers in PVC.

Challenges in bulk isosorbide production from sorbitol is the development of process conditions and catalysts which give a higher yield of isosorbide in the required quality, thus also reducing production-, recovery and purification costs (Werpy, Petersen 2004, p. 60). However, major progress could be accomplished within five years time.

- *Glycols, propylene glycol*. Hydrogenolysis of sorbitol leads to glycols, especially propylene glycol (1,2-propanediol). Propylene glycol is produced by direct hydrolysis of propylene oxide with water in quantities of approx. 9×10^5 t/year. It is an important building block for unsaturated polyesters. It is also used as deicer and automotive antifreeze component. By starting from sorbitol, propylene glycol could be produced from renewable instead of fossil feedstocks.

  This is, however, a medium- to long-term goal. A major challenge is a yield increase from now 35% to at least 60%. This requires the development of efficient catalyst systems with specificity for C-C and C-O bonds and which are also tolerant to catalyst poisoning by components of the biomass sugar substrates.

All in all, sorbitol is assessed as a promising C_6 building block which is produced in bulk quantities already today. In the short to medium term, additional commercial applications of isosorbide can be expected, mainly in the isosorbide modified polymers field, in the solvents area (dimethyl isosorbide) and as speciality plasticizers (isosorbide diesters). In long-term perspective, it bears the potential to provide glycols such as propylene glycol and ethylene glycol from sorbitol.

2.5.3 5-Hydroxymethylfurfural

Production of 5-Hydroxymethylfurfural

5-Hydroxymethylfurfural (HMF) is formally accessible from each hexose or hexulose via acid-catalysed, intramolecular elimination of three H_2O. The preferred substrate is, however, the ketohexose fructose. For fructose, three different routes starting from inulin, starch, or sucrose, respectively, are established for its commercial production (see also section 2.5.1):

- Enzymatic hydrolysis of inulin,
- Enzymatic or acid hydrolysis of starch to glucose syrups, followed by enzymatic isomerization of glucose to fructose with glucose isomerase,

- Acid hydrolysis of sucrose to glucose and fructose, followed by chromatographic separation of glucose and fructose; or enzymatic sucrose hydrolysis by invertase (β-d-fructofuranosidase) from *Saccharomyces cerevisiae*.

Because fructose can be readily obtained on bulk scale by enzymatic isomerisation of glucose, cellulose hydrolysates could, in principle, be also used as feedstock (see also Section 2.5.1).

A major problem in HMF production are the multitude of simultaneous side reactions, partly reversible, partly irreversible, which reduce the HMF yield and complicate its purification. Main side products are humic substances, levulinic acid and formic acid. For the production of HMF, three processes have been investigated in depth, in order to optimise yield versus downstream processing costs (e.g. for HMF purification, solvent recycling) (Kröger 2002).

Process	Advantages	Disadvantages	Stage of development
Reaction in polar organic solvents	In solvent DMSO: Highest HMF yields (> 90%)	Environmentally problematic solvent; Cost-efficient solvent recycling unsolved	Lab stage
	In solvent PEG: PEG and HMF can be more easily separated than DMSO and HMF; Overall more favourable for scale-up than reaction in DMSO	Lower HMF yields (70%)	Lab stage
Reaction in two-phase systems of water/ methylisobutylketon	High HMF yields (90%)	Strongly diluted HMF solutions	Lab stage
Reaction in water	Environmentally friendly, cheap solvent; Potentials for yield improvement not yet exhausted (e.g. through improved catalysts)	Low HMF yields (55%); Strongly diluted HMF solutions	Pilot plant

Table 2-31: Processes for production of 5-Hydroxymethylfurfural from fructose

Use of 5-Hydroxymethylfurfural

HMF possesses molecular features and functionalities which make it an attractive building block for further derivatisation (Kröger 2002), among them

- an aldehyd function,

- a hydroxymethyl group which can be subjected to etherification, esterification, oxidation to an aldehyd group, making the introduction of various groups via C-C bonds possible,
- synthesis of linear polymers from the difunctionalised furan,
- opening up the large industrial group of aromatics,
- conversion to dihydrofuran derivatives by oxidative alkoxylation; from dihydrofuran derivatives, heterocycles such as pyrrols, pyridazines or pyridines can be synthetised.

Table 2-32 gives an overview of promising derivatives of HMF and their potential uses.

Derivative	Potential uses
Products of HMF direct polymerisation	e.g. special phenolic resins
2,5-furan dicarboxylic acid	Bio-based-derived functional substitute of fossil-derived terephthalic acid, use as building-block in polymers analogous to terephthalic acid polyesters Ringopening conversion to adipic acid, replacement in adipic acid derived polymers Reduction and reductive amination to diols and diamines, possibly used as building blocks replacing hexamethylenediamine, *p*-diaminobenzene in polyamides, possibly used as building blocks in new polyesters and nylons Conversion to succinic acid (see Section 2.3.1)
5-hydroxymethyl-furoic acid furandialdehyde 1,6 furandiol 1,6 furan diamine tetrahydrofurandimethanol	Used as building blocks in new polyesters and polyaminesrespectively
Levulinic acid	see Section 2.4.2

Table 2-32: Derivatives of HMF

In the context of BREW, the most promising derivatives of HMF are the difunctionalised

- 5-hydroxymethyl-furoic acid
- 2,5-furan dicarboxylic acid
- furandialdehyde
- 1,6 furandiol
- 1,6 furan diamine
- tetrahydrofurandimethanol

because they bear the potential to be used as building blocks for bulk polyesters and polyamides (Table 2-32). Of special interest is 2,5 furan dicarboxylic acid which can be obtained in a single step by oxidation of HMF. 2,5 furan dicarboxylic acid bears structural similarities to terephthalic acid, the most important aromatic dicarboxylic acid, which is widely used in the production of saturated polyesters, especially polyethylene terephthalate (PET) and polybutylene terephthalate (PBT). Worldwide, terephthalic acid ranked about 25th in tonnage of all chemicals produced in 1992, and about tenth in terms of organic chemicals. In 1992, the world production capacity for terephthalic acid was approx. 12.7 million t/a, and the PET demand approx. 12.6×10^6 t in 1992. 2,5 furan dicarboxylic acid could be a bio-based substitute for fossil-derived terephthalic acid in various polymers, through polymerisation with ethyleneglycol (PET), p-phenylendiamine (KEVLAR), 1,3-propanediol, or trimethylhexandiamine.

To summarize, 5-hydroxymethylfurfural (HMF) is a six-carbon commodity with high industrial potential, and thus, has been termed “a key substance between carbohydrate chemistry and mineral oil-based industrial organic chemistry”. A large number of HMF derivatives can be obtained which – among others – could target the large volume markets of polyesters and polyamides. As of now, only a pilot-plant process has been developed, but HMF is not produced on an industrial scale. This is on the one hand due to its presently high price. If synthetised from crude inulin or fructose (≈1000 €/t), an HMF-marketing price of at least 2500 €/ton arises which compares unfavourably with prices of naphtha and ethylene in the 150 – 400 €/t range (Lichtenthaler, Peters 2004). On the other hand, the water elimination from hexoses has to be considerably improved in terms of yield, higher selectivity and specifity in order to avoid side reactions and by-products. It would be desirable to develop heterogeneous catalyst systems which operate with environmentally friendly and cheap oxidants (e.g. air, oxygen, hydrogen peroxide). Moreover, the catalyst systems must become tolerant to possible poisoning by components of the rather crude biomass hydrolysate feedstock. R&D demand also exists in the use of HMF derivatives in the production of new polymers and their comparative assessment with existing polymers which are to be replaced.

In the long term, it would be favourable if a broad scope of hexoses could be used as feedstock either for HMF production or for the production of related building blocks from other sugars (Werpy, Petersen 2004, p.26ff).

2.5.4 Adipic acid

Production of adipic acid

Adipic acid (hexanedioic acid, 1,4-butanedicarboxylic acid) is commercially the most important aliphatic dicarboxylic acid. In 1999, total worldwide annual capacity for adipic acid was 2.5×10^6 t/a. In large-scale production, the six carbon atoms of the adipic acid backbone are usually derived from benzene, which is hydrogenated to cyclohexane or phenol, which, in turn, is hydrogenated to cyclohexanol. The cyclohexane is then oxidized with air to ketone – alcohol oil (KA oil, a mixture of cyclohexanol and cyclohexanone). Cyclohexanol, cyclohexanone, or KA oil is then oxidised with nitric acid. Moreover, processes for the synthesis of adipic acid from butadiene and carbon monoxide have been developed, but to our knowledge, no commercial plant based on this technology is currently in operation.

Three biotechnological processes have been suggested for the biotechnical production of adipic acid:

- *Biosynthesis of cis,cis-muconic acid from glucose*, followed by catalytic hydrogenation to adipic acid,
- *Biosynthesis of adipic acid from cyclohexanol*. In a patent filed by E. I. du Pont de Nemours and Company,[21] a 17 kb gene cluster was isolated from an *Acinetobacter sp*. that comprises the enzymes which are expected to convert cyclohexanol to adipic acid. Transformation of *E. coli* with this cosmid conveyed the ability to produce adipic acid from cyclohexanol to *E. coli*. No further information on process characteristics are publicly available.
- *Enzymatic conversion of adiponitrile to ammonium adipate by a nitrilase*. With the aim of converting nitriles to carboxylates enzymatically, nitrilases, their gene sequences, and their use in nitril conversion have been patented by Rhone-Poulenc Chimie.[22] No further information on process characteristics are publicly available.

Only the first process will be described in more detail, as it directly involves a biomass substrate: In order to convey the ability to synthetise cis,cis-muconic acid from glucose to *E. coli*, three genes had to be introduced into this host: aroZ and aroY from *Klebsiella pneumoniae*, encoding 3-dehydroshikimic acid dehydratase and protocatechuic acid decarboxylase, respectively, and catA, encoding catechol 1,2-dioxygenase from *Acinetobacter calcoaceticus* (Frost, Draths 1997; Niu et al. 2004; Hasegawa et al. 2000). Different strains yielded 20-37 g/L cis,cis-muconic acid in fed-batch cultures which corresponds to a yield of 15-23% (mol/mol glucose consumed). This is approximately 50% of the maximum theoretical yield of 43% (mol/mol). The theoretical maximum yield could be raised to 86% if a phosphoenolpyruvate (PEP)-

[21] US Patent 6,794,165: Biological method for the production of adipic acid and intermediates (Cheng, Q.; Nagarajan, V.; Thomas, S.M.) (Oct. 2002)

[22] US Patent 5,629,190: Polypeptides possessing a nitrilase activity and method of converting nitriles to carboxylates by means of said polypeptides (Petre, D; Cerbeleaud, E; Levy-Schil, S. Crouzet, J) (May 1995)

independent glucose transport system were used (Niu et al. 2004), but such metabolically engineered cis,cis-muconic acid production organisms have not yet been constructed. However, a shikimate pathway variant has already been constructed which channels PEP preferentially into the shikimate pathway (Ran et al. 2004; Yi et al. 2002). Moreover, yields may be limited by the toxicity of the aromatic intermediates pointing to the likely requirement to reduce their concentration in vivo as well as in the culture broth by metabolic and process engineering (Li et al. 2005). In addition to further optimisations of the production organism, the recovery of adipic acid from aqueous medium at the purity level needed for polymer-grade adipic acid production has yet to be examined. Moreover, further research into the catalytic conversion of cis,cis-muconic acid to adipic acid is required (Thomas et al. 2003).

Use of adipic acid

In 1999, total worldwide annual production capacity for adipic acid was 2.5×10^6 t/a, its consumption in 1995 1.5×10^6 t/a. Its primary application is the production of nylon 6,6 polyamide fibres and resins which accounts for about 80% of the world adipic acid consumption. About 10% are converted to esters for use in plasticizers, lubricants, solvents and in a variety of polyurethan resins. Other uses of adipic acid are as food acidulants, applications in adhesives, insecticides, tanning and dyeing (approx. 8% of consumption).

Derivative, product	World consumption 1995	
	10^3 t/a	%
Nylon 66 fibres	888	59
Nylon 66 resins	329	22
Esters, used as plasticizers, solvents, lubricants	76	5
Polyurethan resins, made from adipic acid polyesters and polyisocyanates	97	6
Miscellaneous (e.g. food acidulant, adhesives, insecticides etc.)	128	8
Total	1,518	100

Table 2-33: Derivatives of adipic acid and their uses (Ullmann's Encyclopedia of Industrial Chemistry, Section adipic acid)

2.6 > C_6 building blocks (derivatives of natural fats and oils)

Production of fats, oils and their main derivatives

World production of natural fats and oils has increased steadily in the last decades. It reached approx. 121×10^6 t in 2002, with approx. 95×10^6 t vegetable oils and 15% animal fats, and is expected to increase to 132×10^6 t until 2012. 80% of these fats and oils are used for human food, approx. 14% of world fat production are used chemically, and 6% as feed material. An increasing share will go into biodiesel production in the coming years. In the chemical use of fats and oils, fatty acids play an important role: The world production of fatty acids from the hydrolysis of natural fats and oils totals about 4×10^6 t per year. For the manufacture of fatty acids on a commercial scale, only fats available in large quantities are used as raw materials, and only the straight-chain $C_8 - C_{22}$ carboxylic acids are of commercial importance.

Figure 2-2 depicts the most important conversion reactions of natural oils and fats. The main products are fatty acids, glycerol, fatty acid methyl esters and fatty alcohols from which other derivates and products are obtained.

There are the following options for biotechnical processes in fats and oil processing to derivates:

- *Production of vegetable oils in GVPs*. Oilseed crop plants are genetically modified in order to increase the oil yield and to tailor the fatty acid profile for certain industrial purposes (e.g. very high content of a given fatty acid in the oil, high content of "rare" fatty acids with industrially interesting properties). More information is given in Section 2.7.5.
- *Single cell oil*. Microorganisms (bacteria, fungi, yeast, algae) have long been known as producers of edible oils which accumulate oils to 50-80% of their dry mass. Such single cell oils could be therefore be derived from an alternative source for oils, other than plant or animal oils and fats. However, for "conventional" fats and oils, fermentative production is not cost-competitive with oil and fat processing from vegetable and animal sources. Up to now, industrial processes have only been established for oils rich in high-value fatty acids, especially polyunsaturated fatty acids (PUFAs) of both the n-6 and n-3 series such as arachidonic acid, docosahexaenoic acid, eicosapentaenoic acid, and (-linolenic acid (Ratledge 1993; Ratledge 2004). These oils or fatty acids, respectively, are used in infant formulas, as ingredient for functional food, or as dietary supplement. Single cell oil could well serve as a source for specific fatty acids which are of interest as high-value oleochemicals if they could be produced in high yields. An understanding of the underlying biosynthetic pathways and genetics of oil accumulation in such microorganisms is essential if lipid yields are to be improved.

- *Enzymatic fat splitting*. Conversion of fats and oils to fatty acids and glycerol or fatty acid methyl ester and glycerol, respectively, by hydrolysis or methanolysis is usually carried out in continuous processes at elevated pressures (2-25 MPa) and temperatures (60-260 °C), with or without catalysts. Both the hydrolysis as well as the methanolysis could also be carried out enzymatically, using lipases or carboxyesterases. The technical feasibility of the enzymatic processes has been demonstrated, but the enzyme cost is too high to allow cost-competitiveness with conventional fat splitting for bulk products. Cost reductions could come from the use of immobilised whole cell biocatalysts and their optimisation by genetic engineering as well as enzyme engineering for high stability towards methanol (see e.g. Fukuda et al. 2001; Bornscheuer et al. 2002).

Economics of oleochemical processes are to a large extent determined by the cost of glycerol which is an inevitable by-product of the conversion of natural fats and oils to derivatives. Therefore, there is a need for new and high-value uses of glycerol in order to make oleochemical reactions economically attractive. For derivatives of glycerol see Section 2.6.

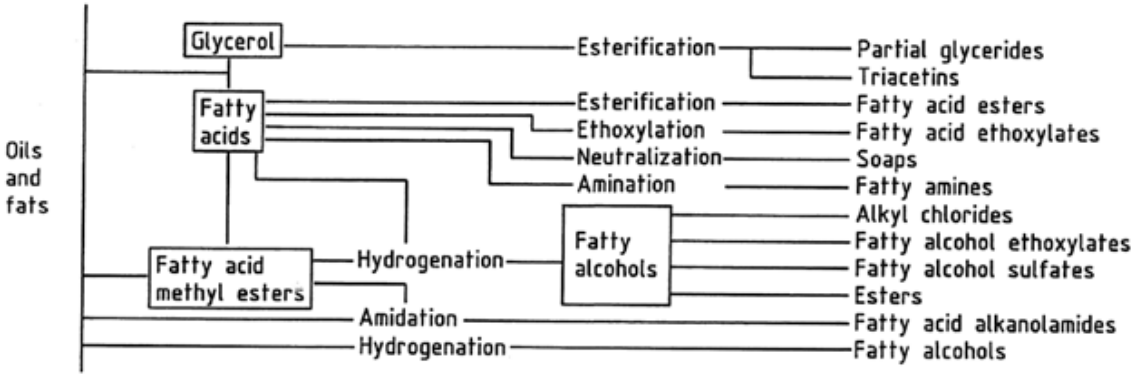

Figure 2-2: Most important conversion reactions of natural oils and fats and products formed (Ullmann's Encyclopedia of Industrial Chemistry, published by Wiley-VCH Verlag GmbH & Co. KgaA)

Use of fatty acids and other derivates of fats and oils

The main derivatives of natural fats and oils are depicted in Figure 2-2, their uses in Table 2-34.

Derivatives	Uses, applications
Fatty acids and derivatives	Metallic soaps, detergents, soaps, cosmetics, alkyd resins, paints; textile, leather, and paper industries; rubber, lubricants
Fatty acid methyl esters	Biodiesel; cosmetics, detergents
Glycerol and derivatives	Cosmetics, toothpaste, pharmaceuticals, food, paints, plastics, synthetic resins, tobacco, explosives, cellulose processing
Fatty alcohols and derivatives	Detergents, cosmetics; textile, leather, and paper industries; duplicator stencils, petroleum additives
Fatty amines and derivatives	Fabric softeners, mining, road building, biocides, textile and fiber industries, petroleum additives
Drying oils	Paints, varnish, linoleum
Castor oil, ricinoleic acid	Polyamide 11, alkyd resins

Table 2-34: Main uses of derivatives of natural fats and oils

Although several lipase-catalysed industrial processes have been operated for several years (see e.g. Liese et al. 2000; Sharma et al. 2001), they are focussed on the resolution of racemic mixtures of chiral synthons and intermediates for the production of fine chemicals, pharmaceuticals and pesticides, and are operated on a multi-kg to multi-ton scale. A lipase-catalysed esterification of palmitic acid or myristic acid to yield isopropyl palmitate or isopropyl myristic acid for cosmetic use is operated on a several-hundred tons scale by Uniqema. Moreover, structured lipids are produced for (functional) food purposes, and research is ongoing for other specialities and fine chemicals uses and chemical modification of the fatty acid chain (e.g. hydrogenation, epoxidation etc) (Tyson et al. 2004). However, biotechnical processes for bulk fats and oils derivatives have not yet been reported, mainly due to the high cost of enzymes (see also oleyl oleate case study by Vicente et al. 2005 in the BREW project).

2.7 Genetically modified crop plants for the production of bulk chemicals

2.7.1 Exploring genetically modified crop plants as production platform for bulk chemicals

Plant-made materials and chemicals have always been used by mankind, and although many plant-based materials and chemicals have been replaced by petrochemically-based ones in the last century, plants still play an important role as sources for materials and chemicals, e.g. by delivering wood for construction, fuel and paper production, fibres (cotton, ramie, hemp, flax, sisal), cork, rubber, carbohydrates such as starch, fats and oils, proteins, as well as a plethora of secondary metabolites (e.g. for use as phytopharmaceutical drugs, for pest control, as flavours and fragrances, as dyes and colorants).
With the development of genetic engineering of crop plants and the foreseeable depletion of fossil feedstocks, genetically modified crop plants (GMPs) are seen as an integral part of a "knowledge-based bioeconomy" (European Commission, DG Research 2004; Genval Group 2004). They are taken into consideration as additional production platform for materials and chemicals for the following reasons:

- Exploitation of the synthetic properties of photoautotrophic organisms, thus harnessing sunlight as energy and CO_2 als carbon source,
- Exploitation of a primary production system, thus being energy and resource efficient,
- Exploitation of crop plants as self-propagating production systems, therefore reduced investment into construction and maintenance of production facilities (as compared to other production platforms such as chemical synthesis or microbial production),
- Use of established agricultural production practices and technology,
- Use of established processing practices and technologies for crop plants for downstream processing after minor adaptations,
- Ease of adaptation to demand of GMP-derived materials and chemicals by alteration of cultivated area.

Adding genetic modification to the tool box expands the possibilities of classical selection and breeding approaches in plant breeding. In order to establish genetically modified plants (GMPs) as additional production platform for plant-based materials and chemicals, the genetic modification approaches can be classified as follows:

- *Optimised delivery of traditional plant-based materials and chemicals,* e.g. wood, cork, lignocellulose and paper/board, fibres (cotton, ramie, hemp, flax, sisal), carbohydrates (e.g. polyglucans such as starch and cellulose, polyfructans such as inulin), rubber, fats and oils, proteins through

  - increased yield,
  - reduced input of production factors (e.g. fertilizer, irrigation, pest control),
  - product profiles which are tailor-made for further industrial use,
  - transfer of industrial processing steps into the crop plant,
  - production in heterologous plant hosts with better agronomic properties than the source plant.
- *Delivery of materials and chemicals, which are traditionally available from other sources than plants*, thus establishing GMPs as alternative production platforms to microbial, mammalian, enzymatic, or chemical production.
- *Delivery of novel materials and chemicals with new or improved functionality.*

Within this section GMPs tailored for reduced input of production factors by introduction of input traits such as herbicide resistance, disease and pest resistance, tolerance towards biotic and abiotic stress (e.g. drought) will not be considered further because they are not specific for GMPs for the production of materials and chemicals. Nevertheless, in future the combination ("stacked traits") of input traits and output traits regarding the production of chemicals and materials in a GMP may be required in order to achieve economically viable production.

2.7.2 Overview of product groups

Although genetic engineering broadens the scope of possible product groups of materials and chemicals that can be produced in crop plants beyond the "traditional" plant-based materials, plant physiology poses limits to the scope:

In order to justify the costs of growing and processing the plant material, the targeted products must be accumulated to high levels *in* the plant. For low molecular weight water-soluble compounds of industrial utility, the osmotic effects of high level solute accumulation place practical limits on how much can be accumulated in the plant. As a consequence, microorganisms are, in general, the preferred production platform for these products if they secrete the compounds into the media. By contrast, high molecular weight soluble compounds which are not significant osmolytes can, in principle, be produced at very high concentrations in some types of plant cells (Somerville, Bonetta 2001).

As a consequence, there is only little overlap of the GMP-derivable product groups with the platform chemicals that have been characterised in the Section 2.1 to Section 2.6 so that microbial and enzymatic processes on the one hand and GMP-approaches on the other hand seem to be more complementary approaches rather than competing ones.

Product groups that are of interest for the production in GMPs are
- Carbohydrates (e.g. starches, fructans, cellulose),
- Fats, oils and fatty acids,

- Industrial enzymes (as enzymes are excluded from the scope of this report, they will not be considered further in this chapter),
- Polymers (e.g. latex, protein-based polymers, polyhydroxyalkanoates),
- Fibres and composites,
- Lignocellulose, and
- High-value, low volume products such as plant-made pharmaceuticals (phytopharmaceuticals, therapeutic proteins, antibodies, vaccines), (functional) food ingredients, flavours, fragrances, secondary metabolites for use as fine and specialty chemicals.

The latter product group of high-value, low volume products will not be covered in this report. Recent further information in this field can be found in e.g. Fischer, Schillberg 2004, Dixon 2005; Fischer et al. 2004; Horn et al. 2004; Joshi, Lopez 2005; Khalsa et al. 2004; Mascia, Flavell 2004; Memelink 2005; Oksman-Caldentey, Saito 2005; Oksman-Caldentey, Inzé 2004; Stoger et al. 2005; Verpoorte et al. 1999; Verpoorte, Memelink 2002; Freese 2002; Herbers 2003; King 2002; Merrigan et al. 2003; Raskin et al. 2002; Tucker 2003; Yan, Kerr 2002; Keil 2002.

An overview of the state of the other product groups will be given in Section 2.7.3. Moreover, they will be described in more detail in the Section 2.7.4 to Section 2.7.8.

2.7.3 State of development of the product groups

GMPs designed for the production of materials and chemicals for industrial use are a subfield of total GMP production. In order to put them into perspective, an overview of GMP production in general is given.

Agricultural commercial production of approved GMPs in general

In most countries, GMPs must be approved in order to be grown on a commercial scale and to be placed onto the market. In 1996, the first approved GMPs were grown commercially. In the nine-year period from 1996 to 2004, the global area, on which GMPs are grown, has risen steadily from 1.7 million hectares in 1996 to 81.0 million hectares in 2004, an increase of more than 47 fold (Figure 2-3). This corresponds to approx. 5% of all global cultivable crop land (1.5 billion hectares). During the period 1996-2004, the accumulated global GMP area was 385 million hectares, equivalent to 40% of the total land area of the USA or China, or 15 times the total land area of the UK (James 2004).

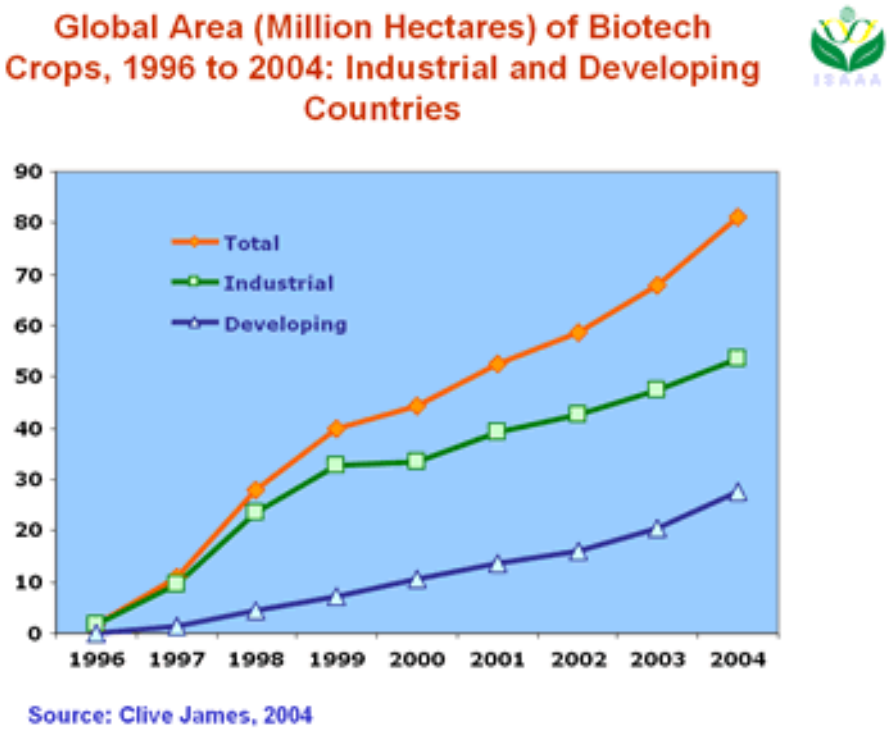

Figure 2-3: Global area planted with approved GMPs (million hectars, 1996-2004)

In 2004, approved GMPs were grown in 17 countries. 14 of them grew GMPs on more than 50,000 hectares (Table 2-35). The most important genetically modified crops are corn (maize), soybean, cotton and canola (rape seed) (Table 2-36), the principal traits are herbicide tolerance, followed by insect resistance, conferred by the Bt toxin, and a combination of both traits (Table 2-37).

In 2004, the global market value of GMPs,[23] was $4.70 billion representing 15% of the $32.5 billion global crop protection market in 2003 and 16% of the $30 billion global commercial seed market (James 2004).

[23] The market value of the global biotech crop market is based on the sale price of biotech seed plus any technology fees that apply.

Country	National GMP area (million hectares)	Share of global GMP area (%)
USA	47.6	59
Argentina	16.2	20
Canada	5.4	6
Brazil	5.0	6
China	3.7	5
Paraguay	1.2	2
India	0.5	1
South Africa	0.5	1
Uruguay	0.3	< 1
Australia	0.2	< 1
Romania	0.1	< 1
Mexico	0.1	< 1
Spain	0.1	< 1
Philippines	0.1	< 1
Total	81	100

Table 2-35: Leading countries in growing GMPs in 2004 (James 2004)

Crop	Total global crop area (million hectares)	Share of GMP area 2004(%)	Share of GMP area 2003 (%)
Soybean	86	56	55
Cotton	32	28	21
Canola/rape seed	23	19	16
Maize/corn	140	14	11
Total	284	29	25

Table 2-36: Principal genetically modified crops in 2004 (James 2004)

Trait	GMP area (million hectares)	Share of total GMP area (%)
Herbicide tolerance	58.6	72
Insect resistance	15.6	19
Herbicide tolerance and insect resistance	6.8	9
Total	81	100

Table 2-37: Principal traits in approved GMPs in 2004 (James 2004)

Agricultural commercial production of approved GMPs for production of materials and chemicals for industrial use

Table 2-37 also shows that output traits in general, and output traits optimising the production of materials and chemicals for industrial use in particular, do not yet play a role in commercially grown GMPs. This is not astonishing, as worldwide only very few GMPs with output traits have been approved for commercialisation (11 out of 74 approved GMPs[24]) up to now (http://www.agbios.com/dbase.php; last accessed May 2005). Out of these 11 GMPs modified in output traits, only 2 are of relevance for the production of materials and chemicals for industrial use. These are

- *Canola lines with increased lauric acid levels*. Two canola lines (*Brassica napus*, lines 23-18-17, 23-198), developed by the company Calgene Inc, have been approved for human consumption (in the form of oil), livestock feed, and industrial applications in the USA in 1994 and Canada in 1996. The GMPs are genetically engineered to express modified seed fatty acid content, specifically high levels of lauric acid and myristic acid. The increased levels of lauric acid in oil from the modified canola lines allow for its use as a replacement for other lauric acid oils, such as coconut and palm kernel oil, in products such as confectionery coatings and fillings, margarines, spreads, shortenings and commercial frying oils.
- *Soybean lines with increased oleic acid levels*. Three soybean lines (*Glycine max*, lines DD-Ø26ØØ5-3; G94-1, G94-19, G168), developed by the company DuPont Canada Agricultural Products, have been approved for human consumption (mostly oil, protein fractions, and dietary fibre) and/or feed use in the USA, Canada, Japan and Australia between 1997 and 2001. The GMPs are genetically engineered to express modified seed fatty acid content, specifically high levels of oleic acid exceeding 80%. This oil is lower in saturated fat, contains no trans-fatty acids, and remains in a user-friendly liquid form. The high levels of oleic acid make the oil more heat-stable for cooking and edible spray applications.

Moreover, dossiers for the approval have been submitted for two additional GMPs, which have, however, not yet been approved (May 2005). These are (Pickardt, de Kathen 2004, p. 13-14)

- *Genetically modified potato with modified starch composition* (at least 98% amylopectin) for the industrial starch production (C/SE/96/3501; Company Amylogene, now BASF, for approval in the EU), and
- *Genetically modified corn with elevated lysine levels* (company Monsanto, for approval in the USA).

[24] The Agbios Database does not contain data from China; the number of approved GVP may therefore be higher, if data from China were included.

GMP field trials

In order to gain additional insights into the R&D pipeline for GMPs for the production of materials and chemicals for industrial use, databases for applications for field trials in the EU (http://biotech.jrc.it/deliberate/gmo.asp und http://gmoinfo.jrc.it/) and the USA were analysed (http://www.nbiap.vt.edu/cfdocs/fieldtests1.cfm). It is not possible to identify unambigiously field trials with GMP for the production of materials and chemicals for industrial use, because of incomplete or confidential business information, or overlap with food, feed and pharmaceutical uses. Nevertheless, approximately 170 applications were submitted for GMP field trials for these purposes in the EU, which is approximately 10% of all field trial applications that were submitted in this period. Table 2-38 gives an indication of the intensity and the level of advancement for the different product groups. All in all, it can be concluded that the main GMP product groups under development, as outlined in Section 2.7.2, are

- Modifications of
  - carbohydrates, especially starch and fructans,
  - fatty acid profiles,
  - amino acid profiles,
  - lignocellulose.
- Development of GMPs as production platform for
  - technical enzymes (not covered further in this report),
  - polymers,
  - miscellaneous products which at present have fine chemical and specialty status, but might attain commodity status in the long term.

The state of development, potential uses and future perspectives will be outlined in more detail in the following sections.

Year	Oil composition	Carbohydrate composition[25]	Industrial enzymes	Lignocellulose, fibres	Novel polymers	Total
1992	1	6				7
1993		10				10
1994	1	5				6
1995	5	11		2		18
1996	7	21	2	2		32
1997	13	7		1		21
1998	1	11				12
1999		19	1	1		21
2000	1	11				12
2001		6				6
2002		6			2	8
2003		1				1
2004	3	13				16
2005[26]		1			1	2
Total	32	128	3	6	3	172

Table 2-38: Applications for field trials with GMP for the production of materials and chemicals for industrial use in the EU, 1992-2005 (Pickardt, and de Kathen, 2004)

2.7.4 Carbohydrates

Overview of GMP approaches for carbohydrate production

The following GMP approaches are taken for the modification of carbohydrate production for industrial purposes:

- Modification of the starch metabolism by
  - alteration of the amylose to amylopectin ratio, construction of GMPs with high amylose or low amylose starch,
  - *in planta* modification of starch properties by alteration of the chain length, the degree of branching, and the phosphorylation pattern of starch,
  - raising the starch yield.
- Modifications of the fructan metabolism by
  - raising the fructan yield, -structure and –properties,
  - heterologous production of fructans in starch or sugar plants.
- Production of novel carbohydrates in GMP.

[25] Data for modified carbohydrate and oil composition may also contain food and feed uses; cannot be unambigiously separated from the publicly available data

[26] Data for 2005 incomplete

Within the field of modifying carbohydrate metabolism, the approaches for the modification of starch metabolism are the most advanced, being on the verge of achieving a more rational design of starches with different functionalities in planta. Moreover, approval of a high-amylopectin potato has been applied for. Modifications of fructan metabolism are not as far advanced as starch metabolism modification, but has already reached the stage of field trials. The focus is on the production of fructans in non-natural fructan-producers such as potato and sugar beet, and on fructan biosynthesis with different functionalities. The production of novel carbohydrates is in the basic research stage with the exception of palatinose-producing GMPs for which a field trial has been applied for in Germany.

Modification of starch metabolism

It is of interest for technological and industrial applications to have available different starches with different properties and functionalities. They are determined by the structure of the starch granules, the ratio of amylopectin to amylose, the degree of branching and the modification by functional groups (e.g. phosphorylation). Starch functionality can be deliberately influenced by the choice of the starch source, and its physical, chemical and biochemical modification. GMPs can, on the one hand, carry out these modifications *in planta* instead of carrying them out in industrial starch processing. On the other hand, novel starch types may become accessible which cannot be efficiently produced by other means. Possible uses for novel starch types, provided they are made available in large quantities at costs comparable with starch, are amylose-ethers which could replace polyethylene and polystyrene in applications where biodegradability is desirable (Somerville, Bonetta 2001).

In the last decade, the core structural and regulatory genes in the starch metabolism pathways have been cloned and functionally characterised in a wide range of species (for recent reviews, refer to Heyer et al. 1999; Schulman 2002; Carrari et al. 2003; James et al. 2003; Jobling 2004; Capell, Christou 2004; Morell et al. 2004; Morell, Myers 2005; Jones 2005). In addition to an improved understanding of starch metabolism in different plants, a number of GMP with modified starch composition and starch properties have been constructed and often also tested in field trials (Table 2-38). This has resulted in an application for commercialisation of a high-amylopectin potato which has been submitted by Amylogene/BASF in the EU and is awaiting approval (Section 2.7.3).

While these GMPs were the result of trials and error rather than of rational design of starches, experts are confident that a more rational design of different starches for industrial purposes in GMPs will become possible the near future (Jobling 2004; Morell, Myers 2005). In principle, the genes and tools are established which allow the generation of diversity regarding genotypes in starch metabolism. What remains to be further developed is the rapid and effective phenotyping of this diversity with respect to

both starch structure and starch function and the elucidation of genotype-structure/function relationships.
Up to now, production of modified starches in GMPs has also been hampered by the fact that synthesis of modified starches often leads to reduced starch yield or pleiotropic effects. In order to make GMPs producing modified starches economically competitive with technological approaches for starch modification, yield increases have to be achieved as well. Several strategies are explored (Capell, Christou 2004) but have so far only resulted in improved starch yields under controlled conditions in the laboratory or greenhouse and on a single plant basis. Their agronomic relevance can only be assessed when similar yield increases can also be achived in open field trials and on a hectare basis (Van Camp 2005).

Modifications of the fructan metabolism

The industrial production of fructans (inulin, inulin neo-series, levan (phlein) and gramminan) in GMPs could be of interest for

- establishing an alternative production process for fructose. Presently, fructose is produced by enzymatic hydrolysis of starch, followed by enzymatic isomerisation (Section 2.5.1). Fructose could also be accessible from fructan hydrolysis, but such processes are not (yet) economically competitive with the starch-based processes,
- production of fructans, especially inulin, as functional food ingredient,
- production of novel fructans with improved functionality (e.g. neo-kestose from neo-inulin (Kilian et al. 2002).

In the last years, several, but not yet all, plant enzymes involved in fructan biosynthesis and degradation have been identified and characterised biochemically. Their corresponding genes have been cloned, and several have been expressed heterologously and their regulation has been investigated. Thus, important prerequisites for a targeted modification of fructan metabolism in plants have been established (Ritsema, Smeekens 2003a; Ritsema, Smeekens 2003b). Bacterial fructan biosynthesis genes turned out to be unsuitable because the GMP yield was significantly depressed. Better results can be obtained with the overexpression of fructan biosynthesis genes of plant origin. However, naturally fructan-producing crops also have efficient fructan-degrading enzymes which significantly reduce fructan yields. Therefore, fructan biosynthesis genes were heterologously expressed in potatoes and sugar beets. However, the achievable fructan concentrations were still much lower (5%) than fructan yields from natural fructan producers such as chicoree (15-20%). Engineering of the properties of the key enzymes fructosyltransferases could provide a solution.

In the EU, applications for at least 16 field trials with GMPs with modified fructan metabolism were submitted, with 6 applications referring to potatoes, 6 to sugar beets, and one application each for chicoree, sunflower, tomato and rape seed.

Production of novel carbohydrates

Several publications relate to the production of carbohydrates in GMP which are normally not produced in plants. These are

- *Cyclodextrins*. Potatoes transformed with a bacterial gene that is involved in cyclodextrin biosynthesis achieved the ability to synthesize cyclodextrins. However, the yields were extremely low (0.001-0.01% of the starch content) (Schulman 2002).
- *Sugar alcohols.* Tobacco transformed with a bacterial gene synthetised the sugar alcohol mannitol. However, these experiments were of basic nature and seem not to be further pursued with the aim to establish a commercial mannitol production with GMPs (Schulman 2002).
- *Palatinose*. Palatinose (Isomaltulose, 6-O-α-d-Glucopyranosyl-d-fructofuranose) is produced on a 60,000 t/year-scale by Palatinit GmbH and is planned to be used as a low-cariogenic sugar replacement (EU approval as food ingredient pending, but expected for 2005). Moreover, it is used as feedstock for the production of isomalt which is obtained from palatinose by catalytic hydration. At present, palatinose is produced by microbial conversion from sucrose to palatinose which is then catalytically hydrated to isomalt. Genetically modified tobacco and potato plants were constructed which quantitatively converted sucrose to palatinose. While the growth of the transgenic tobacco plants was severely impaired, the transgenic potato plants were not affected (Börnke et al. 2002a; Börnke et al. 2002b). An application for field trials with these modified potato plants has been submitted in Germany (B/DE/02/138).

2.7.5 Fats, oils and fatty acids

Plants are a "traditional" source of oils and fatty acids for industrial uses (see also Section 2.6). GMP approaches for the targeted modification of plant fatty acid and oil metabolism have been pursued for more than a decade and are – from a scientific perspective – at least as advanced as GMP approaches for starch metabolism modification. GMP approaches aim at

- increasing the oil and fatty acid yield,
- producing GMPs with oils that have a tailor-made fatty acid pattern for certain industrial applications,
- low cost production of industrial fatty acids that are currently sourced from petrochemicals or from low-yielding crop plants,
- maximising the content of a single, desired fatty acid in the plant oil to shares of more than 80% of the total fatty acids,
- synthetising fatty acids with novel functionalities, such as saturation/desaturation, epoxy- or hydroxy functions.

Major research efforts have been devoted to the tailoring of fatty acid profiles in rapeseed, soybean and sunflower, with the latter two crops mainly modified for food purposes. In rapeseed, modification for industrial purposes was mainly targeted at

modifying the level of erucic acid, stearic acid, oleic acid, myristic acid, and lauric acid. Two GMP with modified fatty acid profile have been approved for commercialisation (high lauric acid canola, developed by Calgene Inc, and high oleic soybean (mainly for food purposes, developed by DuPont Canada Agricultural Products; see Section 2.7.3). Both GMPs have not succeeded in substituting their non-transgenic alternatives, and have therefore not been commercially successful.

Up to now, the principal strategy to modify the fatty acid profile in plant oils was the overexpression or downregulation of those genes which code for the catalytic steps involved in fatty acid synthesis (Thelen, Ohlrogge 2002). It has now become clear that this strategy is insufficient in order to achieve the high levels of single and/or unusual fatty acids in the plant oil required for industrial uses: in most cases the achievable modifications fall behind the yields and concentrations that can be found in wild oil plants or conventionally bred oil plants (Drexler et al. 2003). Moreover, unintended impacts can be frequently found in the GMPs (e.g. reduced oil yield and productivity, enhanced degradation of the fatty acids, impaired germination, unexpected modifications of the fatty acid pattern). As most currently available GMPs do not show significant advantages compared to conventionally bred oil crops, it is unlikely that they can replace conventional oil crops.

In order to reach economically competitive and technologically attractive modified oil compositions, the previous strategy must be complemented by additional approaches to overcome existing limitations: for this to be achieved, the new fatty acids must be efficiently moved from their site of synthesis and channeled through the complex acyl pools to enable their high accumulation in seed oils and their exclusion from membrane lipids. Moreover, the knowledge of the regulatory networks affecting both fatty acid synthesis and primary metabolism has to be broadened. Therefore, attention must be shifted to acyltransferases which will have to be coordinately coexpressed with the fatty-acid biosynthetic genes (Singh et al. 2005).

2.7.6 Amino acids

Several amino acids are produced by biotechnological processes in bulk quantities; they are mainly used as flavour enhancer (glutamic acid) and feed additives (Table 2-29; Kircher, Pfefferle 2001; Dechema 2004; Tryfona, Bustard 2005). The focus of GMP amino acid research is on the essential amino acids lysine, methionine, threonine and tryptophane which limit the nutritional value of certain feeds and major staple food (especially cereals such as wheat, corn, barley and sorghum, which are poor in lysine and threonine, while legumes such as soybean are poor in methionine). GMPs with altered profiles of the above mentioned amino acids do not aim at providing the isolated amino acids. The intention is to provide GMP feeds of improved nutritional value for which the need to add exogeneously produced amino acids has become obsolete. Although conventionally bred crops with modified amino acid contents are available, they have not (yet?) outcompeted amino acids as feed additives due to inferior agronomic properties.

GMPs with elevated levels of certain amino acids have been constructed, and many of them have been tested in field trials. The company Monsanto has applied in the USA for approval for commercial production of genetically modified corn with elevated lysine levels (Section 2.7.3).

Three strategies are employed:

- *Metabolic engineering of the amino acid biosynthetic pathways*. By overexpression of genes for key enzymes and by abolishing feedback inhibition of key enzymes in the respective biosynthetic pathways, transgenic tobacco, corn, soybean and rape seed were obtained which showed elevated levels of the respective amino acid if the synthesis occurred specifically in the seeds (Hesse et al. 2001; Galili, Höfgen 2002; Dewaele et al. 2002; Hesse, Hoefgen 2003). Moreover, the degradation of the amino acid must be inhibited (Arruda et al. 2000; Galili et al. 2001). Up to now, both strategies (enhanced amino acid synthesis and inhibited degradation) have only been combined for lysine synthesis in the model plant *Arabidopsis*, but led to lysine levels which were by a factor of 80 higher than in the wildtype, compared to factors of 5 or 12 for the single strategies (Zhu, Galili 2003). The interaction of plant amino acid synthetic pathways with global regulatory networks is under investigation (Tang, Galili 2004).
- *Expression von storage proteins which are rich in the desired amino acids.* In order to elevate lysine levels, genes for different natural lysine-rich storage proteins, mutated genes with higher lysine codon number and synthetic genes (Forsyth et al. 2005) were overexpressed. Best results were obtained in corn, when a lysine-rich storage protein as well as a feedback-insensitive dihydrodipicolinate synthase were overexpressed in the seed. Lysine levels were raised to 0.7% of seed dry weight, compared to 0.2% in the unmodified plant. It is expected that successful inhibition of lysine degradation in this GMP could make lysine production economically attractive (Galili, Höfgen 2002). Overexpression of S2 albumins is employed in order to achieve elevated methionine levels. However, S2 albumins are major plant allergens (Tsuji et al. 2001; Breiteneder, Radauer 2004) so that the potential allergenicity of the resulting GMP has to be assessed carefully (Shewry et al. 2001; Taylor 2002).
- *Downregulation of synthesis of proteins with nutrionally unfavourable amino acid profiles.* This strategy was realised in corn by downregulation of zein synthesis in the seeds. Zein is a major corn seed protein which is relatively poor in lysine. The overall protein content was unaffected, but the amino acid composition was altered favourably. Agronomic and nutritional properties of this GMP are under investigation (Huang et al. 2004).

If these GMP approaches were successful, they would compete with the fermentative production of the respective amino acids.

2.7.7 Polymers

In addition to starch and fructans (Section 2.7.4) and lignocellulose (Section 2.7.8), the following polymers are being researched for production with GMPs:

- Latex
- Protein-based adhesives
- Protein-based fibres
- Amino acid polymers: polyaspartic acid/cyanophycin.
- Polyhydroxyalkanoates

For all these polymers, R&D is in an early stage of development (see below).

Latex for rubber

Natural rubber (cis-1,4-polyisoprene) is commercially harvested from the Brazilian rubber tree, *Hevea brasiliensis*. Basic research is being conducted to establish molecular genetic tools for *Hevea* and identify the genes involved in *Hevea* rubber biosynthesis. Moreover, experiments are underway to genetically improve, as an alternative source of high quality latex, guayule (*Parthenium argentatum*) in both quantitative and qualitative respects. It is planned to employ metabolic engineering for the production of new types of valued isoprenoid metabolites, such as rubber and carotenoids, and new combinations extractable from the same crop (Mooibroek, Cornish 2000). An application for a small scale field trial with transgenic guayule with modified rubber biosynthesis was submitted in 2000 by the US Department of Agriculture Agricultural Research Service (Pickardt, de Kathen 2004).

Protein-based adhesives

Several protein-based adhesives with interesting properties, such as mussel adhesives, sericin from *Bombyx mori* or Balbiani ring proteins from *Chironomus tendans*, are known and recombinant proteins and synthetic polypeptides with similar properties have been developed (Deming 1999), but are difficult to be produced economically in a functional form (Hwang et al. 2004). In principle, crop plants could be established as production platforms (Scheller, Conrad 2005). However, no relevant publications could be identified.

Protein-based fibres

The following protein-based fibres have been of interest for production in GMPs (Moire et al. 2003; Scheller, Conrad 2005):

- elastin,
- collagen, and
- spider dragline silk.

It has been shown that in principle, elastin-like bioelastic polymers as well as human collagen can be produced in crop plants, but only at very low levels. High level production will require modifications in the amino acid biosynthetic pathways and/or tRNA pools in order to take this production option into consideration for material production for cell culture and biomedical purposes, but also for use in transducers, super-adsorbents and biodegradable plastics (Guda et al. 2000; Moire et al. 2003; Scheller, Conrad 2005).

For spider dragline silk proteins, expression and purification systems for plant-based silk proteins have been developed (Scheller et al. 2004; Scheller, Conrad 2004), but the selection of suitable sequences for defined applications and commercialisation is still at an early stage. Moreover, there are no reports of the successful spinning of plant-derived silk proteins (Scheller, Conrad 2005). Because the properties of spider silk depend heavily on the way the material is spun (Lazaris, et.al. 2002), advances in artificial spinning technologies will be crucial for the further development and application of silk-like fibres produced in plants (Moire et al. 2003; Scheibel 2004).

Amino acid polymers

Polyaspartic acid is produced by chemical synthesis (see also Section 2.3.3), but could also be made available from the cyanobacterial polymer cyanophycin. The ability for cyanophycin biosynthesis was conferred to tobacco and potato and improvements in cyanophycin accumulation were achieved by chloroplast expression and enhancement of amino acid biosynthesis (Neumann et al. 2005). However, this will have to compete with bacterial production systems (Frey et al. 2002). No reports of synthesis of poly-γ-glutamate or poly-ε-lysine in transgenic plants could be identified.

Polyhydroxyalkanoates

Polyhydroxyalkanoates (PHAs) are naturally occurring energy and carbon storage polymers which can be synthetised by many bacteria. PHAs have material properties similar to those of some common plastics such as polypropylene, and have therefore been proposed as biodegradable and bio-based alternatives to petrochemically based polymers, but cannot be produced yet in a cost-competitive way.

For nearly fifteen years, attempts have been made to establish PHA biosynthesis in GMPs. Since 1992, a spectrum of PHAs ranging from the stiff PHB to the more flexible copolymer P(HB-HV) to mcl-PHAs have been synthetised in plants (Poirier 2001; Poirier 2002). Moreover, PHA synthesis has been used to modify cotton and flax fiber properties in planta (John, Keller 1996; Wrobel et al. 2004).

Most experiments were carried out in the model plant *Arabidopsis thaliana*, but also agronomically more relevant crops such as maize, sugar beet and *Brassica napus* were

used. The dedicated PHA company Metabolix Inc. (USA) favours switchgrass (*Panicum virgatum*) for PHA production (Snell, Peoples 2002). In maize and rape seed, PHA levels of up to 8% PHA/dw were achieved. However, model calculations show that levels of approx. 15% PHA/dw must be achieved for an economically viable process.

Challenges for the future lie in further increases in the level of accumulated PHAs and at the same time avoiding side effects of overproduction, such as chlorosis, male sterility, growth retardation, and overall yield depression. In addition, stability of the trait over several generations must be demonstrated. Moreover, efficient downstream-processing procedures must be developed. For economically viable processes, a several-purpose use of the PHA-producing GMP is envisioned: after extraction of the PHA, further use of the residues for feed or energy production is planned, but has not yet been investigated in more detail (Moire et al. 2003; Scheller, Conrad 2005).

2.7.8 Lignocellulose

Wood is an attractive and widely used raw material for fibre, chemical, and energy production. Its major component is lignin. The composition and structure of lignin limits the technological use of wood. Therefore, strategies for lignin modification are of considerable interest: by downregulation of lignin biosynthesis, by modification of its composition and structure, an enhanced adaptation of lignocellulosic material to downstream conversion processes is to be achieved.

Since the beginning of the 1990s, the biotechnological and molecular genetic toolbox has been developed which allows the modification of cell wall structures by genetic engineering: It comprises the in vitro propagation of trees, somatic embryogenesis for mass clonal propagation, efficient gene transfer systems for conifers, soft- and hardwoods, the cloning and characterisation of many lignin biosynthetic genes, the possibility to alter the expression of several genes simultaneously by stacking or transcription factors, and a broadened understanding for lignin biosynthesis (Merkle, Dean 2001; Halpin, Boerjan 2003; Boudet et al. 2003).

In the past decade, research focussed on a handful of genes involved in cell wall formation (Table 2-39), and transgenic plants with altered expression of one or more lignification genes in both model and economically important species were constructed.

Trait	Gene
Biomass yield	GA-20 oxidase, glutamine synthetase, 4-coumarate-CoA ligase
Fibre length	GA-20 oxidase
Lignin content	4-coumarate-CoA ligase
Lignin composition	Ferulate-5-hydroxylase, cinnamyl alcohol dehydrogenase
Cellulose	4-coumarate-CoA ligase

Table 2-39: Traits and genes for lignin modification (Halpin, Boerjan 2003)

Preferred plants are poplar, but also *Pinus*, *Eucalyptus* and the ambertree (*Liquidambar styraciflua*). It could be shown that modification of lignin content, composition, or both is in principle achievable. Structural analyses have shown that plant cell walls can tolerate large variations in lignin content and structure. In some cases, the potential value for agriculture of transgenic plants with modified lignin structure has been demonstrated:

- *Pulping performance.* Transgenic poplars with downregulated cinnamyl alcohol dehydrogenase (CAD) and altered lignin structure or with downregulated caffeate/5-hydroxy-ferulate O-methyltransferase (COMT), resulting in reduced lignin content, were grown for four years and then tested for their performance in Kraft pulping for paper making. The reduced-CAD lines had improved characteristics, allowing easier delignification, using smaller amounts of chemicals (- 6%), while yielding more (+ 2-3%) high-quality pulp. Tree growth or fitness was not impaired (Pilate et al. 2002).
- *Feedstock for ethanol production.* Transgenic poplars with downregulated cinnamyl alcohol dehydrogenase (CAD) are more easily hydrolysed by *Clostridium* cellulases, resulting in twice as high release of sugars from the transgenic lignocellulosic material than from unmodified controls (Dinus 2001; Dinus et al. 2001; Boudet et al. 2003).

In the coming years, thanks to functional genomics, new target genes of both plant and microbial origin will rapidly become available, and their combined and coordinated expression and its impact on lignin structure and properties will be examined. A major challenge will be the establishment of rapid and reproducible techniques for the detection of chemical and structural cell wall alterations in order to establish genotype–lignin structure relationships (Boudet et al. 2003).

The number and hectareage of field trials with lignin-modified transgenic trees has increased in recent years. Principal investigators are the Michigan Technology University, and ArborGen, a joint venture of several companies, among them International Paper, Fletcher Challenge Forests and Westvaco Corp. They belong to the largest paper- and wood-processing companies, and have invested 60 million US-$ into the development of transgenic trees in recent years (Pickardt, de Kathen 2004).

Environmental impacts of transgenic trees are an issue of intensive scientific and social debate.

2.7.9 Challenges for using GMPs as production platform for bulk chemicals

It has been shown that GMPs can – in principle – be used as production platform for a large variety of chemicals and materials, among them also bulk chemicals. However, in many cases, GMPs would have to compete with existing or emerging alternative production platforms. In order to become competitive, solutions to the following challenges must be developed:

- Still too low yields and levels of the desired chemicals and materials. The simultaneous modification of several genes and of interrelated metabolic and regulatory networks will be required.
- Unintended and pleiotropic effects of the genetic modifications,
- Cost-effective downstream processing,
- Need to reduce time to transgenic production organism and to first product samples (e.g. by transient expression with viral systems),
- Need to reduce time to full-scale production and market,
- Establishing integrated product concepts with multiple uses of the GMP biomass (e.g. extraction of target substance, use of residues as feed, for energy etc.) while at the same time complying with regulatory requirements.

Compared to other production platforms, GMPs have a disadvantage with regard to time to market due to compliance with regulatory requirements: for GMPs, field testing is mandatory, as well as a product approval before market entry. Moreover, regulatory requirements for the co-existence with non-transgenic food and feed production as well as forestry (in the case of modified trees) are under development.

2.8 Summary and Conclusions

Aim

It is the aim of Chapter 2 to assess the technological potential of biotechnology for the production of bulk chemicals in order to contribute to answering the question to which extent, how and when biotechnology will play a role in this field. This is the first part of the more comprehensive assessment in the following chapters where additionally environmental, economic and market, safety and perception issues are taken into consideration (Chapter 3-6). In this context, this Chapter 2

- gives an overview of bulk chemicals which could be produced by means of biotechnological processes from biomass,
- identifies and characterises promising bulk chemicals with respect to their stage of development, market attractiveness and challenges for their further development,
- provides a basis from which chemicals for further assessment in the following chapters were chosen,
- puts White Biotechnology and Green Biotechnology approaches for the production of bulk chemicals into perspective.

Specificities of biotechnical bulk chemical production

Although several overviews of the technological potential of biotechnology in industrial chemical production have recently been published (see e.g. OECD 1998; OECD 2001; Liese et al. 2000; Straathof et al. 2002, Hüsing et al. 2003, Werpy, Petersen 2004; Lorenz, Eck 2005; Marscheider-Weidemann, Hüsing 2004 to name but a few), they do not adequately cover bulk chemicals. Rather, their main focus is on pharmaceuticals, fine and speciality chemicals, where biotechnology has already taken root and is expected to expand considerably in the short to medium term (Straathof et al. 2002; Figure 2-4).

However, the production of bulk chemicals from biomass differs in many challenging aspects from the biotechnological production of fine and specialty chemicals (Table 2-40), e.g. large production volumes, low product prices, long-running processes, higher importance of process than product innovation, competition against well-established, optimised chemical processes. Moreover, assessing the potentials of biotechnology in the production of bulk chemicals from biomass is highly uncertain because it is generally assumed to be a long-term development with gradual implementation until 2050. This process is expected to be driven by the progressive depletion of fossil resources, increasing competitiveness of renewable feedstocks and increasing environmental pressure. In addition, it implies a paradigm shift in the underlying chemistry: from the conversion of hydrocarbons to the conversion of carbohydrates, thus requiring fundamentally different chemical reactions and processes.

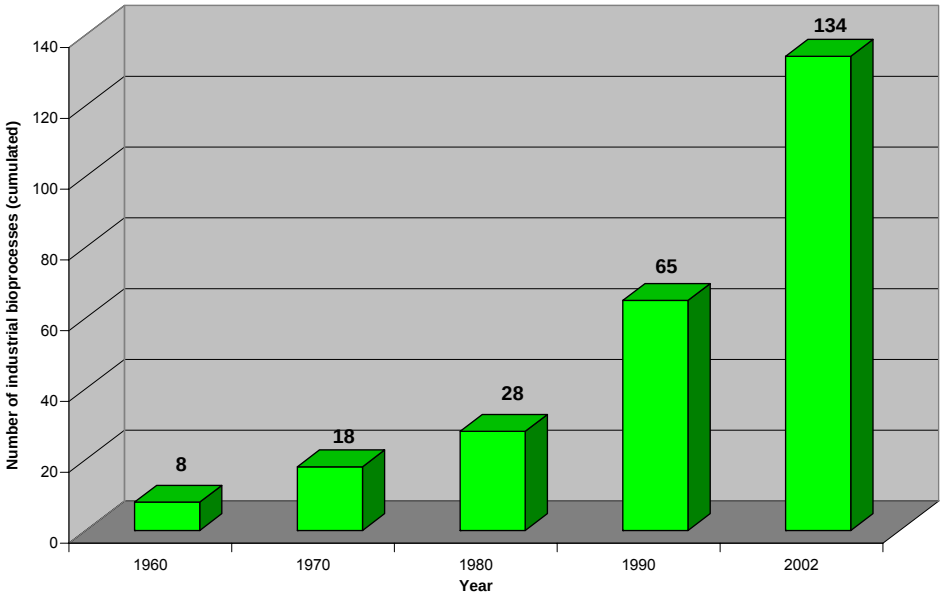

Figure 2-4: Cumulative number of industrial biotransformation processes implemented on industrial scale (data from Straathof et al. 2002)

	Bulk chemicals	Fine Chemicals
Production volume	Large	Small
Product prices	Low	High
Profit margins	Low	High
Process/ product life cycle	Long	Short
Chemistry	Simple	Advanced
Innovation	Process	Product
Competition	Cost	Performance

Table 2-40: Differences between bulk and fine chemicals

Technological potential of biotechnology for bulk chemical production and actual production today

Against this background, in this chapter an overview of the technological potential of bio-based bulk chemicals was prepared for the first time.[27] In a first screen, an extensive list of possible bio-based chemicals was compiled (see Figure 2-1, Tables 2-28, 2-29). It was found that several bio-based chemicals are produced on bulk scale[28] already today (Table 2-41), with ethanol, glucose, fructose, L-glutamic acid, sorbitol, citric acid, and L-lysine even above

[27] Werpy, Petersen 2004 also do address bulk chemicals, but their main focus is on promising candidates for an integrated biorefinery which produces fuels, high-value chemicals, materials and power from biomass.

[28] Bulk scale was defined here as an annual production volume of at least 20-50 kt worldwide.

200 kt/year worldwide.[29] This is in contrast to the wide-spread notion that biotechnology is not suitable for bulk chemical production. On the other hand, the products listed in Table 2-41 only account for a minor amount of total chemical production; and the main use of the above-mentioned bulk chemicals produced in amounts > 200 kt/year is in the food, feed and fuel sector, but not as chemicals. It implies that substantial scientific-technical progress has to be made in order to expand bio-based bulk chemicals in the coming decades.

Bio-based chemical	Annual World Production (million t/a)	Building block
Ethanol	32	x
Glucose	5-20	x
Fructose	10.1	
Acetone	3 (historical, abandoned)	
L-Glutamic Acid	1.5	
1-butanol	1.2 (historical, abandoned)	(x)
Sorbitol	1.1	x
Citric Acid	1.0	
Glycerol	0.75 (not biotech)	v
L-Lysine	0.7	
Furfural	0.2-0.3 (not biotech)	v
Acetic acid	0.19 (fermentation)	x
Lactic acid	0.15*)	x
Polylactic acid	0.14*)	
Propionic acid	0.13 (including non-biotech processes)	
Gluconic acid	0.1	
Vitamin C	0.08	
Alkylpolyglycosides	0.05-0.07	
L-Sorbose	0.05	
Xanthan	0.04	
Sugar alcohols, e.g. erithritol	0.03	
L-Threonine	0.03	
Vitamin B2	0.03	
Malic Acid	0.025	

x: building block as defined at the beginning of Chapter 2; v: studied in Chapter 2

*) Capacity data (not production)

Table 2-41: Bio-based chemicals produced on bulk scale (> 20 kt/a) already today

Identification and characterisation of building blocks of key importance for transition from petrochemicals to bio-based bulk chemicals

The extensive list of possible bio-based chemicals (see Figure 2-1 and Tables 2-28 and 2-29) was subjected to further assessment by a product-tree approach as described in the introduction to Chapter 2, in order to identify building blocks of key importance for a possible

[29] In historical perspective, 1-butanol and acetone were also produced in this order of magnitude. Moreover, glycerol and furfural are produced in bulk amounts from biomass; however, biotechnological processes do not play a role in their industrial production.

future transition from petrochemicals to bio-based bulk chemicals.[30] This led to the selection of 19 building blocks plus derivatives of natural fats and oils as representatives for complex products. These products have been discussed in detail in Chapter 2.1 to 2.6. In addition, genetically modified crop plants were discussed in Chapter 2.7. These are, however, not within the focus of this report which deals, in first instance, with White Biotechnology (fermentation and enzymatic conversions). The products covered in Chapter 2.1 to 2.6 include 5 chemicals which are abundantly available from biomass, i.e. glycerol, xylose/arabinose, levulinic acid, furfural and lignins. Since biotechnological processes are not necessarily involved in these latter processes, they partly fall outside the scope of this project and are therefore not followed up in this report. The remaining building blocks (ethanol, acetic acid, lactic acid, 3-hydroxypropionic acid, 1,3-propanediol, acrylic acid, succinic acid, fumaric acid, aspartic acid, 1-butanol, 1,4-butanediol, glucose, sorbitol, 5-hydroxymethylfurfural, and adipic acid) were subjected to further evaluation by the industry and academic partners in the BREW project. The purpose of the evaluation was to take into account the chances of large-scale industrial production in view of possible competition among each other and competition with petrochemical products. This led to the exclusion of certain products from the further analysis, i.e. 3-hydroxypropionic acid, fumaric acid, aspartic acid, 1,4-butanediol, glucose, sorbitol and 5-hydroxymethylfurfural. At the same time, it was concluded that a few more products should be included, namely citric acid, caprolactam, lysine, polyhydroxyalkanoates (PHA), hydrogen and acrylamide. The reasoning leading to the inclusion of these additional products was very diverse: Citric acid was included in spite of its irrelevance as non-food bulk chemical because it can serve as benchmark for aerobic fermentation processes, given the extensive experience that has been made with this product in the last decades. Caprolactam hardly features in scientific literature and therefore was not included in the review in Chapter 2. If successfully produced by fermentation it could, however, enter industrial production very quickly, thereby leading to substantial changes in the supply chain of polyamides. Lysine is currently used as feed additive (outside the scope of this report) but if prices could be reduced substantially it could serve as building block for bio-based polymers. For polyhydroxyalkanoates (PHA), not only research is ongoing for the production in living plants (Green biotechnology; see Chapter 2.7.7) but they are already produced on commercial scale by fermentation (compare Crank et al., 2005). Hydrogen is primarily seen as energy commodity but it also plays an important role in hydrogenation and hydroformulation processes leading to industrial chemicals. Finally, acrylamide is included with its production route via enzymatic conversion of acrylic acid (the alternative production from acrylic acid and 3-hydroxypropionic acid has been mentioned earlier in this chapter). While this process does not strictly fall into the scope of this report due to current petrochemical production from acrylonitrile, its inclusion was motivated by the large scale of the enzymatic production.

Table 2-42 provides an overview of the compounds (ordered by number of carbon atoms) which have been selected for in-depth analysis in Chapter 3 and 4 of this report (see second column from the right). There is some correspondence between these selected products and those identified by Werpy and Petersen (2004; see first column from the right and footnote to Table 2-42). The difference between the two product lists is mainly caused by different terms of reference. Within the BREW project, the aim was to identify bulk chemicals produced by biotechnology from biomass, whereas Werpy's and Petersen's (2004) objective was to identify top value added chemicals from biomass sugars within the concept of an integrated

[30] A similar approach had also been chosen by Werpy, Petersen 2004.

biorefinery which produces fuels, high-value chemicals, materials and power. Moreover, the difference between the two assessments reflects the rather broad range of possible outcomes as a consequence of incomplete and uncertain data. Therefore, the choice of building blocks presented in this chapter also reflects the subjective assessments of the BREW project team in 2005 which may be subject to change over time. It should also be stressed that the focus was on carbohydrate- and oil-derived bio-based chemicals. Additional efforts beyond the scope of this project should be taken to identify opportunities for e.g. nitrogen-containing compounds and aromatics.

Strategies

The selected building blocks can be distinguished according to the prevailing strategy for their market entry (termed "strategic fit criteria" by Werpy, Petersen 2004). We distinguish **four strategies the first two of which** play a key role in decision making. These are:

- *Direct substitution of a bulk petrochemical.* This strategy implies that a bulk chemical which is presently produced from petrochemical resources would be substituted by an identical substance, produced from biomass with the help of biotechnology. The substitute could either be the building block itself (e.g. fermentatively produced acetic acid replaces petrochemical acetic acid, likewise for PDO), or a derivative of the building block (e.g. 1,2-propanediol obtained by hydrogenation of fermentatively produced lactic acid replaces petrochemically derived 1,2-propanediol; ethylene is obtained from bio-ethanol instead of steam cracking of naphtha). Advantages of this strategy are that the markets for these products already exist and the market drivers are well known, which substantially reduces the uncertainty. On the other hand, the bio-based products have the disadvantage to have to compete on a cost basis against processes which have been optimised for a long time, and which often run on depreciated capital.
- *Functional competition of bio-based bulk chemicals with fossil-based ones*. When making the transition from petrochemical to bio-based production, it will not always be necessary or possible to provide the same product. Rather, a comparable or even superior functionality could be provided. (e.g. bio-based polylactic acid could functionally replace fossil-based PET, PS or PP; PTT made from bio-based 1,3-propanediol could replace nylon and PET; organic solvents could be replaced by bio-based ethyl lactate). Cost-competition with petrochemicals becomes less important

No	Number of carbon atoms	Building block	Chosen for further analysis in this project	For comparison: TOP47 candidates identified by Werpy, Petersen 2004 *)
1	0	Hydrogen	x	x
2	2	Ethanol	x	x
3	2	Acetic acid	x	x
4	3	Lactic acid	x	x
5	3	3-Hydroxypropionic acid		x (among top 12)
6	3	1,3-propanediol	x	(y)
7	3	Acrylic acid	x	(y)
8	3	Acrylamide	x	(y)
9	4	Succinic acid	x	x (among top 12)
10	4	Fumaric acid		x
11	4	Aspartic acid (chem use)		x
12	4	1-butanol	x (with byproduction of ethanol and acetone)	x (also acetone)
13	4	1,4-butanediol		(y)
14	6	Sorbitol		x
15	6	5-Hydroxymethylfurfural		
16	6	Adipic acid	x	x
17	6	Citric acid	x	x
18	6	Caprolactam	x	(y)
19	6	Lysine	x	x
20	complex	Natural fats and oils derivatives	(x) (fatty acids, oleyl oleate, monoglycerides)	
21	complex	Polyhydroxyalkanoates (PHA)	x	(y)

x: included/chosen y: included as derived/additional product but not among TOP47

*) Additional TOP47 candidates identified by Werpy and Petersen (2004) which are not included in this table are: Formic acid, methanol, carbon monoxide, carbon dioxide, acetaldehyde, glycine, oxalic acid, ethylene glycol, ethylene oxide, alanine, glycerol, malonic acid, serine, propionic acid, acetoin, aspartic acid, fumaric acid, malic acid, threonine, arabinitol, furfural, glutamic acid, glutaric acid, itaconic acid, levulinic acid, proline, xylitol, xylonic acid, aconitic acid, ascorbic acid, fructose, 2,5 furan dicarboxylic acid, glucaric acid, gluconic acid and kojic & comeric acid.

Table 2-42: Overview of identified building blocks, their choice for further analysis in the project, and comparison to findings from Werpy, Petersen 2004

if a new or improved functionality can be provided which either allows the competition with established, proven products, or the opening of new applications. Within this strategy, two substrategies can be distinguished:

- *Proven product.* The substitute could be a proven product (e.g. fossil-based 1,3-propanediol is substituted by bio-based 1,3-PDO; fossil-based ethyl lactate is substituted by bio-based ethyl lactate). This substrategy partly overlaps with the strategy "direct substitution of a bulk petrochemical", but differs from it as it often also allows new or broader uses of the proven product. As the product is already proven, the market risks are reduced.
- *New product.* The substitute could be a new product. Examples are new polymers based on succinic acid as building block instead of fossil-derived dicarboxylic acids; 2,5-furan dicarboxylic acid as a biomass-derived functional substitute of fossil-derived terephthalic acid, or isosorbide diesters as new speciality plasticizers. Advantages are new market opportunities and no direct competition from petrochemical routes. Drawbacks lie in the not-yet-defined market and the requirements of substantial amounts of capital and time to develop it.

A given compound can be both an example of *direct substitution* and *functional substitution*. For example, bio-based PDO can replace petrochemical PDO (direct substitution) but it can also functionally replace another compound, e.g. for its solvent properties. PTT is also an example of both a direct and a functional subsititution: PTT made with bio-based PDO can be substituted for PTT made with petrochemically based PDO (direct substitution); but PTT made with bio-based PDO can also replace PET or nylon polymer, depending on the application (functional substitution).

The **third and the fourth strategy** generally are of subordinate importance but they can certainly influence the final decision. They are:

- *Bio-based building blocks as basis of interesting product trees.* In this strategy, bio-based building blocks could give rise to a large product portfolio when further processing (conventional chemical or biotechnical processing) is applied, and could therefore be needed in bulk quantities. In this option, the market risks inherent in the first two strategies could be reduced because of the broad product portfolio. It depends on the chemical whether either the route from biomass to the building block or from the building block to its derivatives, or both, is presently seen as the main bottleneck. In general, the route from biomass to the building block is the bottleneck if the building block at the same time aims at direct substitution of a petrochemical bulk chemical (e.g. ethanol, 1-butanol, adipic acid). While biological transformations account for the majority of routes from biomass to building blocks, chemical transformations predominate in the conversion of the building blocks to their respective product portfolio. Promising candidates for this strategy could be e.g. lactic acid, succinic acid, levulinic acid, or sorbitol.
- *Importance for valorisation of all biomass constituents.* A commercially viable bulk chemicals production from biomass requires the valorisation of all constituents of the biomass feedstock. Abundant constituents which on the one hand require valorisation and on the other hand bear the potential to form the basis of an interesting product portfolio are glycerol, xylose/arabinose, levulinic acid, furfural and lignins.

Stages of development

Another approach for mapping opportunities is to categorize products/processes according to the stage of development. In accordance with the Stage-Gate® process by Cooper,[31] the following stages were distinguished: idea (1), feasibility (2), pilot stage (3), commercialisation (4). The application of this approach shows that both the full list of the building blocks in Table 2-42 and those selected for further analysis cover all stages:

- *Idea*. For example, acrylic acid as well as acetic acid and 1,4-butanediol are mainly in the idea stage.
- *Feasibility*. Research into the feasibility of biotechnological bulk production is, among other productss, underway for 3-hydroxypropionic acid, succinic and fumaric acid, 1-butanol, 5-hydroxymethylfurfural, and adipic acid. The development of *biotechnical bulk* processes for natural fats and oils derivatives, lignins, aspartic acid for chemical use, xylose/arabinose, and levulinic acid is also in this stage in many cases.
- *Pilot stage.* The stage of pilot processes has, for example, been achieved for ethanol from lignocellulosic feedstocks, furfural (involving no biotechnical process), glucose from lignocellulose, and hydroxymethylfurfural.
- *Commercialised.* Commercialisation has been achieved for ethanol from glucose, sucrose and starch as feedstock, acetic acid for food use, lactic acid, 1,3-propanediol from glucose, aspartic acid for food use (mainly aspartame production), glucose from starch, sorbitol and others. The following building blocks are commercialised, but without using biotechnological processes: glycerol, levulinic acid, furfural, lignins. Commercial biotechnological production of 1-butanol was abandoned in the 1980s.

Feedstocks

All commercialised processes for building block production presently rely on glucose, sucrose or starch as feedstock. Moreover, the majority of fermentation processes in the feasibility stage also start from these feedstocks. A less advanced process (pilot plant stage) is the conversion of lignocellulosic feedstocks to fermentable sugars such as glucose, xylose and arabinose and their further conversion to the target chemical.

The use of lignocellulosic feedstocks would be desirable for reasons of availability, cost, valorisation of all constituents of biomass and environmental impacts (see following chapters).

Due to strongly increasing production of biodiesel for fuel use in the coming years, its by-product glycerol will become available in large amounts at low price. Within a strategy of glycerol valorisation, it could also be used as carbon and energy source in fermentative processes.

Although White Biotechnology in general does not require feedstocks from genetically modified plants (GMP), synergies between White and Green Biotechnology could be exploited provided the GMPs deliver feedstocks which allow a more cost-effective production

[31] http://www.prod-dev.com/stage-gate.shtml

of bio-based chemicals. GMPs with altered agronomic properties ("input traits"), resulting in increased yield or reduced need for pesticides, irrigation, or fertilizer as well as GMPs with biomass tailored in such a way that it is more amenable to conversion to fermentable sugars or contains lower amounts of difficult-to-valorise substances would both support the economic and environmental performance of White Biotechnology processes. Taking the present stage of development and commercialisation of GMPs into account, carbohydrates and vegetable oils from commercially grown herbicide- and insect-resistant GMPs are readily available. Up to now, no GMPs with tailored biomass constituents have been approved for commercialisation and are grown on a substantial scale – these GMPs are still in the feasibility and field testing stage.

Role of Green Biotechnology and its interplay with White Biotechnology

Presently, it is a controversial issue in White and Green Biotechnology stakeholders' discussions what the role of Green Biotechnology and its interplay with White Biotechnology could and should be. Safety and perception issues play a substantial role in these discussions and will be dealt with in depth in Chapter 5 and 6.

It has already been pointed out in the previous paragraph that synergies between the two fields could be exploited if Green Biotechnology delivered biomass feedstocks at lower costs (e.g. due to improved agronomic properties and reduced input of production factors) or improved quality (e.g. higher yield of desired biomass constituents, ease of conversion to fermentable sugars, fewer by-products) than can be obtained from conventional crops.

For most low-molecular weight, water-soluble chemicals of industrial utility, microorganisms are, in general, the preferred production platform if they secrete these chemicals into the medium whereas the osmotic effects of high level solute accumulation put plant-based production platforms at a comparative disadvantage. As a consequence, for the majority of the building blocks identified in this Chapter 2, White Biotechnology and GMP approaches seem to be more complementary than competing ones.[32]

The situation may be different especially for complex products of high molecular weight which are not significant osmolytes and could therefore be accumulated to high levels in the GMP. The genetic modification of crop plants bears the potential to transfer synthetic and processing steps - which could as well be done in bioprocesses – into the GMP, thus establishing competition between White and Green Biotechnology approaches. Examples could be

- Production of modified carbohydrates, such as modified starches, novel fructans or modified cellulose,
- Establishing alternative production processes for fructose: hydrolysis of polyfructans from GMPs could compete with enzymatic isomerisation of starch hydrolysates,

[32] There may be exceptions, e.g. chemicals which do not need to be isolated from the plant for further use, such as the essential amino acid lysine, used as a feed additive to improve the nutritional value of animal feed. Presently, lysine is commercially produced by microbial fermentation with a world production volume of 700 kt/year. GMPs with elevated lysine levels could well present a competition to fermentatively produced lysine for feed use in the future.

- Establishing alternative production processes for derivatives of natural oils by in- planta synthesis,
- Production of novel polymers in planta (e.g. PHAs, protein-based fibres, amino acid polymers).

Compared to microbial production platforms, GMPs have, however, a disadvantage with regard to time to market due to compliance with regulatory requirements: for GMPs, field testing is mandatory, as well as product approval before market entry. Moreover, regulatory requirements for the co-existence with non-transgenic food and feed production as well as forestry are still under development.

3. Environmental and economic assessment of 21 products[33]

In this chapter we present the methodology and the results of the detailed analyses on the environmental impacts and the economics of 21 chemicals that could potentially be produced in bulk quantities via White Biotechnology. The functional unit, for which we present the results in this chapter (Chapter 3) is one tonne of organic chemical, while scenario projections for Europe as a whole (EU-25) will be given in Chapter 4. In contrast to some earlier reports a uniform methodology and a common database for all relevant processes is used in this study in order to ensure comparability of the results. This concerns, for example, agricultural production, the conversion of crops to fermentable sugar, auxiliaries, steam and power production and waste management. As much input data as possible used in the calculations are reported, with the exception of confidential information provided by the partners or originating from purchased databases, e.g. Ecoinvent. The selection criteria for the products and processes covered in this chapter are (see Table 3-1):

- The White Biotechnology process (fermentation, enzymatic conversion) must either be reported in literature to be feasible or it must be deemed feasible by the project consortium.
- The availability of basic data (e.g., on the stoichiometry of the fermentation process) is another prerequisite for eligibility. Preferably in-depth knowledge should be available among the project partners.
- The products studied must have the potential to be used in bulk quantities (if not now, then at least of the boundary conditions change).

According to the original plans of this project, only **proprietary data** were going to be used for modelling the bio-based chemicals. In order to enlarge the number of products and to extend the temporal scope into the future, the so-called **Generic Approach** was developed and applied. The Generic Approach is defined here as a method which allows to estimate, *ex ante*, the environmental impacts and basic economic features of new biotechnological processes for which pilot plant or lab scale data do not yet exist or for which process data are not publicly available because they represent sensitive information. The Generic Approach has been applied to both processes representing the current state –of –the art and for future processes. For these two categories one or more different process schemes have been assumed for the separation and purification of the products (see Table 3-1). In total, 95 process schemes have been evaluated.

Around 60% of the products shown in Table 3-1 are produced by fermentation (No. 1-13). Four products each are manufactured by enzymatic conversion (No. 14-17) and by chemical conversion of White Biotechnology products (No. 18-21). Some of the products, namely ethanol and hydrogen, are also common fuels but they have been included here in their role as chemical intermediates. Ethanol, moreover, represents a benchmark for anaerobic fermentation with several decades of industrial experience. By analogy, citric acid has been included as model case of an aerobic process; citric acid is studied exclusively for this purpose

[33] The authors of this chapter are Dr. Martin Patel and Barbara Hermann (M.Sc.), Utrecht University, Department of Science, Technology and Society (STS) / Copernicus Institute, Utrecht, Netherlands. Many other partners of the BREW project have contributed methodological concepts and data which were crucial for the preparation of the text in its current shape.

while it will not be used as bulk chemical next to its common use as food ingredient. Lysine, an amino acid, is a widely known as animal feed but it could also be used as bulk chemical intermediate (e.g., for polymer production) if the prices were low enough. As shown in the lower part of Table 3-1 we studied also a few more products that can be derived from White Biotechnology by means of a chemical conversion step. The products covered belonging to this category are polylactic acid (PLA; from lactic acid), ethyl lactate (from ethanol and lactic acid), ethylene (from bioethanol) and polytrimethylene terephthalate (PTT; from 1,3-propanediol and petrochemical terephthalic acid).

The majority of all cases given in Table 3-1 are based on the Generic Approach. Proprietary data from companies and research institutes play an important role to validate the outcome of the Generic Approach. This holds also for data from the PEP review reports by SRI which were made available by the industrial partners for the purpose of this project. SRI reports have been used for ethanol (SRI-PEP2000-7), 1,3-propanediol (SRI-PEP227), acrylic acid (SRI-PEP 2003 6D), lactic acid (SRI-PEP96-7), succinic acid (SRI-PEP236), citric acid (SRI-PEP188B), lysine (SRI-PEP97-8 and SRI-PEP97-9), PHA (SRI-PEP2002-8), acrylamide (SRI-PEP91-3-3) and polytrimethylene terephthalate (SRI-PEP227).

Product group		Product	Number of White Biotechnology cases/flowsheets			Data from companies & research institutes *)
			TODAY	FUTURE	Total	
Alcohols	1	Ethanol	3	3	6	UCM
	2	1,3-propanediol (PDO)	7	2	9	DuPont, Degussa
	3	ABE (Butanol)	2	4	6	
Carboxylic acids	4	Acetic acid	2	4	6	BP/A&F
	5	Acrylic acid	0	1	1	
	6	Lactic acid	2	5	7	NatureWorks, Shell
	7	Succinic acid	2	4	6	
	8	Adipic acid	1	2	3	
	9	Citric acid	3	1	4	
Nitrogen compounds	10	Caprolactam	0	1	1	
	11	Lysine	3	1	4	
H_2	13	Hydrogen	1	0	1	A&F
Polymer	12	PHA	9	3	12	A&F
Products of enzymatic conversions	14	Fatty acids	1	1	2	Uniqema
	15	Oleyl oleate (biolubricant)	1	1	2	UCM, Uniqema
	16	Monoglycerides	1	1	2	UCM, Uniqema
	17	Acrylamide	1	1	2	Degussa
Products derived from WB chemicals*)	18	Ethylene (from bioethanol)	1	1	2	
	19	Ethyl lactate (from ethanol & lactic acid)	1	4	5	
	20	Polylactic acid (PLA; from lactic acid)	2	5	7	
	21	Polytrimethylene terephthalate (PTT; from PDO & pchem. terephthalic acid)	7	2	9	
		Total	**50**	**47**	**97**	

*) Most cases are based on the Generic Approach. In addition, the companies listed in this column provided proprietary data.

Table 3-1: Overview of the number of processes and data source for the White biotechnology products studied in the BREW project

3.1 The Generic Approach

In this chapter we explain the methodology of the Generic Approach, which has been developed and applied to assess the bio-based products. The purpose of the Generic Approach is to estimate the environmental impacts and basic economic features of new biotechnological processes for which process data are not available. The Generic Approach has been applied both processes representing the current state of the art and for future processes. It consists of the following steps:

- First, a process flow diagram is prepared for each process scheme. The process flow diagram is prepared at the level of process steps and consists of the following sections:
  - Seed train (production of microorganism)
  - Fermentation/bioprocess
  - Filtration
  - Product workup (several steps)

  As an example, the process flow diagram of 1,3-propanediol is shown in Figure 3-1. The material inputs to the system are fermentable sugar, water, nutrients and process chemicals such as solvents. The output of the system studied in the Generic Approach is the chemical studied. In terms of system boundaries, the Generic Approach hence represents a *gate-to-gate analysis* (of the chemical plant; the extension to *cradle-to-gate* and to *cradle-to-grave* is subject of Chapter 3.2). For all compounds, the mass flows are estimated which represents a very time intensive step of the Generic Approach. Important aspects related to the preparation of the process flow diagram will be explained below separately for the biotechnological step (fermentation or enzymatic processes, Section 3.1.1) and for product separation (Section 3.1.2).
- Second, based on the material flows through each process step, the total energy use of the system studied in the Generic Approach is estimated (see below, Section 3.1.3).
- Third, again based on the material flow balance, the investment cost of the total system is estimated. This calculation step was performed by DSM, where the so-called *Functional Unit Method* (*FUM*) has been developed (DSM, internal document) using in-house expertise and process studies (e.g., SRI studies). The investment cost is further processed in a calculation applying standard business economics which is not part of the Generic Approach and will be explained in Chapter 3.3.

The process flow diagrams of all process schemes are given in Appendix A9. The diagrams differ mostly with regard to the product separation and purification stage.

3.1.1 Fermentation processes

The "philosophy" of the Generic Approach, as applied to biotechnological processes in the BREW project, is that the **upper limits (horizon values)** of the key parameters concentration, productivity and yield can be derived from biotechnological processes for which research, development and industrial practice can look back on an experience of many years. These are

a) ethanol production as representative of anaerobic processes and
b) citric acid as representative of aerobic processes.

In view of the process data for these two products and the experience made in the BREW consortium with other products it is assumed in this study that **substantial R&D in the next 2-3 decades** would allow to reach

- **a product yield of about 90 mol-% of the theoretical value**
- **a maximum productivity of 10-20 g/l/h in the case of aerobic processes and 50 g/l/h for anaerobic processes**
- **concentration values** that are around current end-of-batch values.

These assumptions are applied to all types of fermentable sugars. This includes not only C_6 sugars which are nowdays commonly produced from starch crops (i.e., starch which is converted to dextrose) and from sugar crops (i.e., sugar beet and sugar cane which contain saccharose) **but also C_5/C_6 sugars** (i.e., mixtures of glucose, xylose and other sugars) as they can be produced from lignocellulosic feedstocks (i.e., woody biomass such as maize stover). With the exception of ethanol, R&D nowadays deals primarily with the conversion of C_6 sugars (esp. dextrose) to desired chemicals. The direct conversion of C_5/C_6 sugars to the target molecules would hence require additional efforts in R&D. However, the BREW partners consider the achievement of such a target to be feasible in the medium to longer term.

Based on these assumptions and making use of expert judgements from the project team, the process parameters for the FUTURE as shown in Table 3-2 have been established. The values for the yields for the FUTURE have been derived from the stoichiometric equations shown in Table 3-3. These stoichiometric equations account for the electron balance of the matabolism involved. The data for the FUTURE in Table 3-2 are based on the assumption that future designs will always involve a continuous fermentation process. Moreover, differences in present-day productivities and concentration (reported in Table 3-2 in the rows for TODAY) have been taken into account for estimating the respective process parameters for the future. The process data representing the current state of the art originate mainly from literature and partly also from experts in the BREW consortium.

It should be noted that the data for concentration, productivity and yield shown in Table 3-2 have a large influence on the final outcome of the environmental and the economic calculations. For a few products (especially 1,3 propanediol and lactic acid) it has been possible to compare the calculation results for TODAY performed with the Generic Approach with company data from pilot plant or industrial facilities (these data were provided by BREW partners). According to this comparison (for energy use) the calculations according to the Generic Approach reflect well the current processes (compare below Section 3.4.2, 3.4.3 and Appendix A8 - A10). However, it should be kept in mind that only very few of these comparisons could be made for TODAY and no such basis for comparison exists for the FUTURE. For the datasets for the FUTURE, an attempt was made to ensure internal consistency of the values across the products in order to ensure a comparable level of technology. However, this is a very difficult task and other experts may consider some data for the FUTURE in Table 3-2 to be too ambitious or too conservative (for example, some experts may find the assumption made for FUTURE concentrations to be too conservative for continuous fermentation designs while the assumptions for FUTURE productivity and yields might be considered by some to be too optimistic). Sensitivity analyses for productivity showed (at the example of ethanol) that marginal improvements beyond a certain threshold value (e.g., around 10 g/l/h for ethanol) hardly change the results, i.e. the results for energy

use and for the economics of FUTURE processes with productivities of 10g/l/h and 50 g/l/h respectively differ by less than 5% (see Box 3-3, Section 3.4.4).

Apart from concentration, productivity and yield Table 3-2 also contains values for plant capacities. As a default, a size of 100 kt p.a. has been assumed. This accounts for technical limitations for upscaling of fermentors and the resulting limited benefits in terms of economies of scale. On the other hand, according to one large-scale producer involved in the BREW project, clear economies of scale can also be expected beyond a capacity of 100 kt p.a. Therefore, larger capacities are assumed for sensitivity analyses for some chemicals (Table 3-2). These larger values do not take into account whether transportation distances, storage and other logistics may be prohibitive to a scale-up of this extent.

Product		Broth concentration (g/l)	Productivity (g/(l*h))	Yield (g product/g substrate)	Plant capacities (kt p.a.) Default	Sensitivity
1 Ethanol	TODAY anaer.	100	2.2	0.46	100	
	FUTURE anaer.	130	50	0.47	100	**400**
2 PDO	TODAY Aer.	100	1.67 - 6	0.41	100	
	FUTURE Aer.	100	15	0.54	100	**200**
3 ABE (Butanol)	TODAY anaer.	20	0.36	0.42	100	
	FUTURE anaer.	45	15	0.50	100	200
4 Acetic acid	TODAY anaer.	18	0.15	0.50	100	
	FUTURE anaer.	50	15	0.90	100	**400**
5 Acrylic acid	FUTURE anaer.	50	10	0.72	100	200
6 Lactic acid	TODAY anaer.	160	5	0.93	100	
	FUTURE anaer.	180	20	0.95	100	**300**
7 Succinic acid	TODAY anaer.	80	1.8	0.88	100	
	FUTURE anaer.	150	15	1.01	100	**300**
8 Adipic acid	TODAY Aer.	20	0.42	0.17	100	
	FUTURE Aer.	40	10	0.47	100	200
9 Citric acid	TODAY Aer.	150	5	0.86	100	
	FUTURE Aer.	150	10	0.96	100	(no sens. calc.)
10 Caprolactam	FUTURE Aer.	see Lysine (precursor)	6.2	0.39	100	200
11 Lysine	TODAY Aer.	100	1.7	0.34	100	
	FUTURE Aer.	140	10.0	0.63	100	(no sens. calc.)
12 PHA	TODAY Aer.	150	3.0	0.35	100	
	FUTURE Aer.	200	10.0	0.43	100	200
HORIZON VALUES	FUTURE anaer.		max. 50	90% (mol) of theoretical		
	FUTURE Aer.		max. 10-20	90% (mol) of theoretical		

Table 3-2: Assumptions for concentration, productivity and yield of fermentation processes based on glucose for TODAY and the FUTURE in the Generic Approach

Note 1: Citric acid is included in the table above because it is industrially produced in large-scale industrial facilities applying aerobic fermentation technology. The data for citric acid are hence important to put the other data in perspective while not having any relevance for the large-scale future production of chemicals for non-food purposes.
Note 2: The assumptions for enzymatic processes are not included in Table 3-2; they are discussed separately in Chapter 3.4.3.
Note 3: The assumptions made for further processing of White Biotechnology chemicals by means of chemical processing are neither reported in Table 3-2.

Product	Equation	References
Ethanol	$C_6H_{12}O_6 \rightarrow 2\ C_2H_6O + 2\ CO_2$	Bender, 2000
PDO	$C_6H_{12}O_6 + 0.31\ O_2 \rightarrow 1.42\ C_3H_8O_2 + 1.73\ CO_2 + 0.32\ H_2O$	SRI 1999 (PEP 227)
ABE (butanol)	$C_6H_{12}O_6 \rightarrow 0.20\ C_3H_6O + 0.82\ C_4H_{10}O + 0.08\ C_2H_6O + 1.50CO_2 + 12\ H_2$	Generic Approach, based on Qureshi 2001a,b
Acetic Acid	$C_6H_{12}O_6 \rightarrow 3\ C_2H_4O_2$	Klemps 1987
Acrylic Acid	$C_6H_{12}O_6 \rightarrow 2\ C_3H_4O_2 + 2\ H_2O$	Straathof, 2005
Lactic Acid	$C_6H_{12}O_6 \rightarrow 2\ C_3H_6O_3$	SRI 1998 (PEP 96-7)
Succinic acid	$C_6H_{12}O_6 + 2\ CO_2 + 4\ "H" \rightarrow 2\ C_4H_6O_4 + 2\ H_2O$	SRI 2001 (PEP 236)
Adipic Acid	$3\ C_6H_{12}O_6 + 7\ O_2 \rightarrow 2\ C_6H_6O_4 + 6\ CO_2 + 12\ H_2O$	Linton & Nisbet 2000
Citric Acid	$C_6H_{12}O_6 + 0.5\ O_2 \rightarrow C_6H_8O_7 + 4\ H$	Generic Approach
Caprolactam	$C_6H_{12}O_6 + (NH_4)_2SO_4 + O_2 + 3\ H_2 \rightarrow (CH_2)_5CONH + 5\ H_2O + H_2O_2 + NH_4OH + HSO_4^-$	based on Lysine
Lysine	$C_6H_{12}O_6 + (NH_4)_2SO_4 \rightarrow C_6H_{14}N_2O_2 + HSO_4^- + 3\ H_2O + 2\ O$	based on SRI 1999 (PEP 97-8)

Table 3-3: Stoichiometric equations for the products studied with the Generic Approach

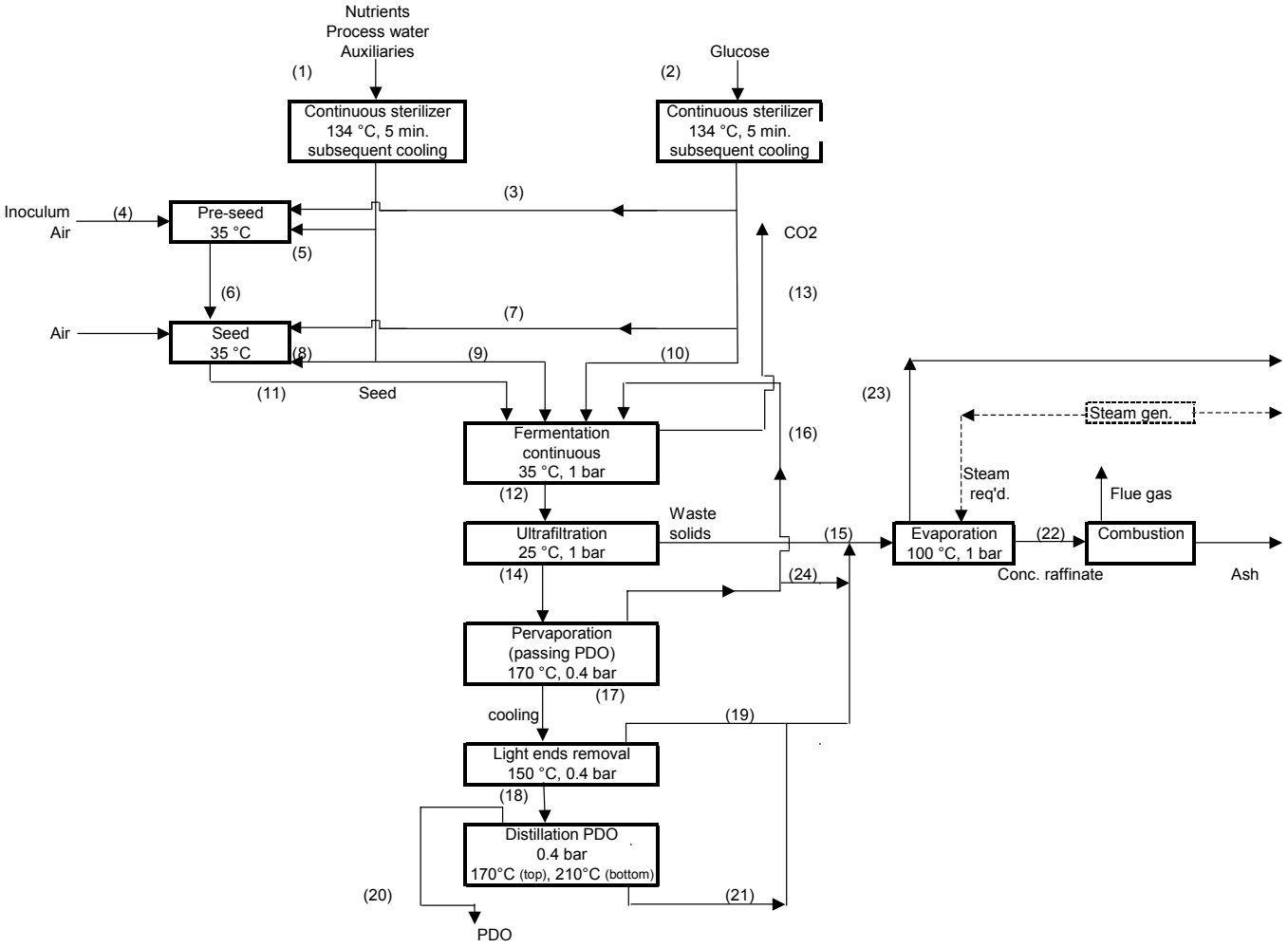

Figure 3-1: Example of a process flow diagram of 1,3-propanediol (PDO) as developed for the Generic Approach (Case for FUTURE with pervaporation of PDO)

3.1.2 Product separation

For each product studied with the Generic Approach, at least one process scheme each has been designed for the present and future for the product separation and purification. The schemes included in Appendix A8 to A10 represent a selection from a larger number of process flow diagrams which have undergone screening by the project partners. For the FUTURE, more process schemes were developed than for TODAY in order to account for the wider range of options due to (possible) technology development (see Table 3-1). Regarding the options for the FUTURE the following considerations led to the configurations proposed:

- Separation processes based on precipitation, which involve the input of large amounts of chemicals and lead to low-value byproducts (such as gypsum) and/or wastewater with high salt loads, are not considered to be viable for large-scale production in the FUTURE. Other separation processes based on temperature increase, membranes and/or extraction are therefore chosen for the FUTURE.
- Extraction is treated as a fully acceptable option for the FUTURE in spite of the general trend in the last 2-3 decades to avoid solvents wherever possible for reasons of health, safety and environment. The reason for inclusion of extraction among the separation processes is the potential use of "green solvents" with clearly lower impacts (e.g., in terms of carcinogineity and toxicity). Besides extraction, solvents are also commonly used for adsorption; with the same reasoning as for extraction, also adsorption is considered as a fully acceptable option.
- Membrane processes are taken into account as an option due to their (expected) low energy use and the avoidance of high salt loads as required for precipitation.[34] The membrane processes taken into account are selective hydrophobic membranes, hydrophilic membranes, pervavoration and electrodialysis. Some membranes which have been assumed in the process flow diagrams of certain products do not exist nowadays; successful R&D would be required in order to make them commercially available within the timeframe studied.
- The avoidance of salt loads also makes electrodialysis an attractive option for the future. The high power requirements are considered acceptable in view of on-site electricity production from biowaste streams.

When modelling the mass flows in product separation and purification a number of important assumptions and simplifications have been made:

- It is assumed that *all* fermentable sugar entering the fermenter is converted to the main product, byproduct(s) or to biomass, i.e. no fermentable sugar is assumed to be present in the effluent of the fermenter. In practice, this is unlikely to be the case, i.e. some additional measures will probably need to be taken in product separation and purification in order to ensure the required purity of the product.
- Regarding the part of the sugar that is *not* converted to the main product and the byproduct(s) we assume that

[34] Among the membrane processes, reverse osmosis is an exception since water is the permeate, i.e. both wanted and unwanted products end up in the retentate. Since this is not desirable, separation processes based on reverse osmosis are not taken into account.

  - for aerobic processes, two thirds are converted to biomass and the remaining third is oxidised to CO_2;[35]
  - for anaerobic processes, half is converted to biomass while the other half is oxidised to CO_2.
- In all process flow diagrams, the biomass (solid) is separated from the product stream by means of an ultrafiltration step that immediately follows the fermentation. The biomass is dried and is then used for raising steam.
- Process water is recycled wherever possible in order to avoid excessive consumption.
- Solid products are dried and packaged while liquid and gaseous products are not packaged because it is assumed that different quantities of the products will be used/sold, in accordance with current practice. The difference in energy use and investment costs, is, however, negligible.
- Pervaporation processes have been assumed in some process flow diagrams for the FUTURE However, a significant amount of research will often still be necessary to put this process into use on an industrial scale.
- Bleed/purge streams were generally set at 5% if no details were available on the size of the flows.

3.1.3 Process energy

The process energy for the system covered in the Generic Approach is determined by multiplying, for each process step, the throughput by the specific energy use. A distinction is made between fuel use (combustibles), steam and power. The data used are based on an extensive literature search (among others, by Isaac, M., 2004). A summary of the chosen data by type of process step is given in Table 3-4. The full overview of the literature data on which this selection is based can be found in Appendix A4.

As shown in Table 3-4 the amount of energy required for evaporation differs decisively depending on the number of evaporation stages. In our model calculations, we assume that single-stage evaporation is used as long as the water to product ratio (before evaporation) is smaller than 5:1 (see above). Beyond this ratio, double-effect evaporation is assumed. The higher investment costs of double-stage evaporation compared to single stage evaporation are taken into account in the economic analysis. In a real industrial facility further options for optimization typically exist, e.g. heat integration by use of Pinch Technology and imports and exports of heat from other processes. These options are not taken into account in our analysis since it would require a higher level of detail.

Among the processes that are particularly uncertain with regard to their energy use are the membrane processes such as pervaporation which are nowadays not yet commercially available and, in particular electrodialysis. With respect to the latter, uncertainty stems from the fact that most publications offer electricity use relative to the amount of product. However, with electrodialysis, the energy consumption depends on the amount of substance transferred and thus on the relative concentrations before and after the process step. For simplicity, we have assumed a generic value for the energy that is necessary to transfer one

[35] This estimate is based on detailed calculations on the carbon splitting of 4 anaerobic and 4 aerobic fermentation processes. The aerobic processes have ratios around 1:2.
For anaerobic processes the spread is much larger; since less metabolic CO_2 should be formed than for aerobic processes we assume a ratio of 1:1.

unit of product in order to reach the higher concentration (Table 3-4). We do account for double acids that have two charges that will need to be transferred. However, it is uncertain to what extent such a generic energy value can accurately represent the specific characteristics of the various products.

	Unit	Chosen	Range
Fermentation			
Sterilization	kg steam/kg ferm. medium	0.1	0.1 - 0.8
Agitation	kW/m^3 of fermentation	0.5	0.1 - 12
Aeration	kW/m^3 vvm	2.5	4 - 6 0.2 - 2
Agitation and Aeration	kW/m^3	3	1 - 5
Separation			
Centrifugation	kWh/m^3 feed	1.5 7	0.7 - 2.5 6.2 - 25
Membrane Filtration			
- Microfiltration	kWh/m^3 permeate	2	1.2 - 2.6
- Ultrafiltration	kWh/m^3 permeate	5	3.5 - 16
- Diafiltration	kWh/m^3 permeate	5	5
- Nanofiltration	kWh/m^3 permeate	7	1 - 7
- Reverse osmosis	kWh/m^3 permeate	9	2.5 - 10
Distillation	kg steam/kg product MJ$_e$/kg product	see below*) -	0.9 - 4.4 0.07-0.14
Electrodialysis	kWh/eq.	0.1	0.07 - 0.34
Evaporation, single stage	kg steam/kg evap. kWh/kg evap.	1.2 0.04	0.005 - 1.4 0.04
Evaporation, multi-stage	kg steam/kg evap. kWh/kg evap.	0.1-0.5 (depends on stages) 0.005	0.01 - 1.25 0.002 -0.0344
Drying	kg steam/kg evap. kWh/kg evap.	1.5 0.1	0.24 - 3 0.1 - 1
Refrigeration	kWh refrigeration /kWh power	4.25 2.5 1	

*) Estimation of energy use for distillation by multiplying the heat of evaporation by a reflux factor of 1.3. The heat requirements of the distillation column may be reduced substantially by vacuum. Electricity demand to generate vacuum can be negligible (see sheet "Vacuum").

Table 3-4: Specific energy consumption per process step (for background data see Appendix A4)

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3.2 Methodology of the environmental assessment

Quantitative analyses on the environmental impacts related to bio-based bulk chemicals produced by White Biotechnology are scarce and fragmented. Results have been published – usually in the form of isolated case studies – by producers (e.g., NatureWorks; see Vink et al.

2003 and Vink et al., forthcoming a and b), research institutes, consultancies and international organizations (e.g., OECD 2001). The problem related to the use of these studies is that, being prepared by different organizations, they lack consistency in terms of basic data and key assumptions. To overcome this problem and in order to generate results that are comparable across products, an assessment tool has been developed, which is called BREWtool and which allows to conduct economic assessments (see Chapter 3.3) next to environmental assessments.

The environmental assessment performed with BREWtool follows the principles of a life cycle assessment (ISO 1997-2000) by studying the entire system starting from the extraction of resources such as crude oil and from agricultural production to the final product and its waste management (for further details on system boundaries see below). For the comparative evaluation of the bio-based chemicals, functionally equivalent or, wherever possible, chemically identical petrochemical products are used.

BREWtool is a spreadsheet-based (MS Excel) tool developed by Utrecht University. It is taylored to the assessment of bio-based materials. The novelty and the features of the bio-based products and underlying biotechnological processes studied in BREW limits the usefulness of commercial LCA software tools (e.g., SimaPro, GaBi and Umberto; LCL 2004) and partly even makes them impractical to use for our purposes. The main reasons are the lack of data for numerous raw materials, auxiliaries and chemicals in commercial tools, the limitation to a few indicators only in BREW (see Section 3.2.1; this makes it unnecessary to work with extensive datasets covering a large number of emissions), allocation procedures (Section 3.2.3) and energy and emission credits (Section 3.2.4); moreover, a spreadsheet-based (MS Excel) tool allows to link directly and quite easily the LCA calculations with the Generic Approach, with the economic assessment (Section 3.3) and with the scenario projections (Chapter 4). The structure and use of BREWtool is described in Appendix A7.

3.2.1 Goal and Scope of the environmental assessment

Apart from the economic analysis, the purpose of BREWtool is to assess the environmental effects of substituting bio-based chemicals for petrochemicals. We now discuss the key features of BREWtool with regard to functional unit, system boundaries and the environmental impact categories.

Functional unit
The functional unit used in this study is **one tonne of product** at the factory gate. The functional unit describes the purpose of the product system studied. In BREW, a considerable number of bulk chemicals is analysed, each of which could subsequently be used in many different secondary processing steps and numerous end use applications. Thus for reasons of pragmatism the more general functional unit of one tonne of bulk product has been chosen. As for the reporting of impact categories, it should be recognised that comparisons made at this level may lead to distortions if important parameters differ decisively at the end use level (e.g., the amount of the chemical required to fulfill a certain function).

System Boundaries
In BREWtool, environmental assessments are conducted both for the system “cradle-to-factory gate” and “cradle-to-grave”(see Figure 3-2). The system “cradle-to-factory gate” has the advantage that more results are available in open literature for this system boundary, thus allowing to make comparisons (e.g., comparison with LCA on petrochemical products

published by APME; Boustead, 1999-2005). The system "cradle-to-grave" has the advantage that it is comprehensive with regard to the steps in the process chain, i.e. it includes also the use phase and the management of post-consumer waste (see Figure 3-2). The use phase, which is part of the system "cradle-to-grave", is usually identical for comparable bio-based and petrochemical chemicals (e.g., a given plastic component in a passenger car) and in most cases, it does not lead to emissions. The use phase is therefore neglected in this study.[36] Emissions from the use phase do, however, occur during *dissipative* use of chemicals (e.g., release of solvents from paints in open application or antifreeze agents). In this study the resulting emissions (CO_2) are fully accounted for in the environmental analysis for the system "cradle-to-grave".

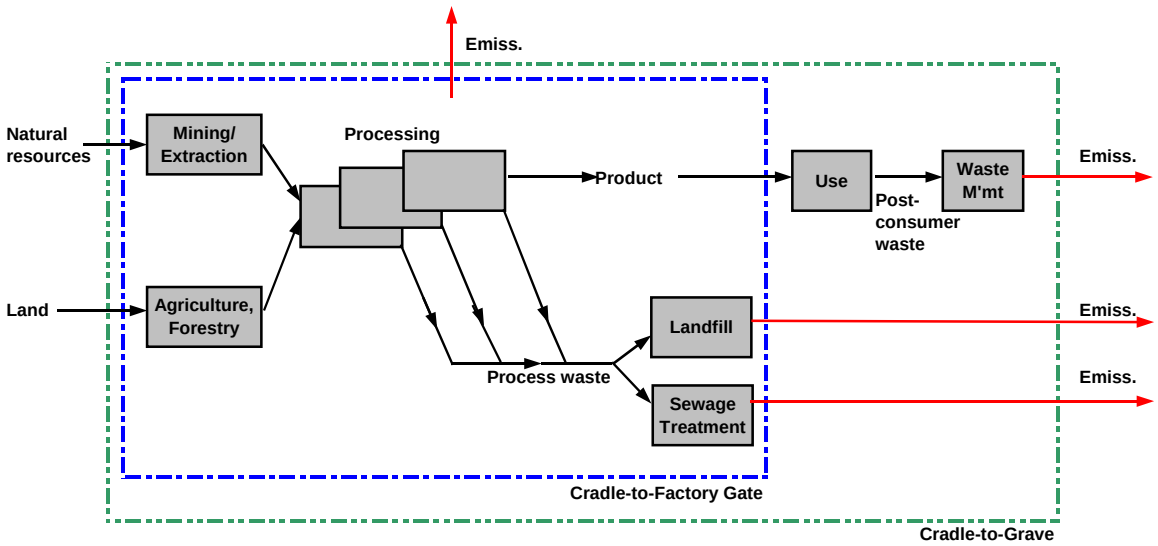

Figure 3-2: System and systems boundaries in life cycle assessment (LCA)

Subsystems

The systems "cradle-to-factory gate" and "cradle-to-grave" consist of a number of subsystems, which are indicated by the grey boxes in Figure 3-2. Each subsystem consists of one or more process step/unit operations. The subsystems included in BREWtool are listed in Box 3-1 and are explained as follows:

- The subsystem **"Agriculture/forestry, biomass pretreatment and conversion" (No. 1)** includes fermentable sugar originating from crop plants grown in Europe (maize and lignocellulose) and also fermentable sugar from sugar cane which grows only in tropical countries. Fermentable sugar from sugar cane is included because its production costs are much lower than the other two options and because it is attractive with regard to non-renewable energy use, greenhouse gas emissions and land use. In contrast, fermentable sugar from sugar *beet* is not included among the options because its production costs are clearly higher than all other options.

  Instead of using maize, other starch crops can also be used. In Europe, wheat is another very common source for starch. Due to the relatively high price of wheat gluten by-product it may be economically more attractive to produce starch-based fermentable

[36] Very small sources of emissions are neglected such as the diffusion of plasticizers from the matrix to the surface of a plastic component in a passenger car.

sugars from wheat instead of maize. However, other aspects also need to be taken into account such as soil conditions and crop rotation which may speak for sourcing starch also from other crops apart from maize and wheat. In the BREW project it has not been studied which starch crop(s) may be preferred and for which reason. Instead, the production of fermentable sugar from maize is chosen as a valid respresentative.

The production of fermentable sugar from sugar cane and starch crops (and also from sugar beet) has been operated on large scale for several decades and the technology is widely available and mature. In contrast, the production of sugars from lignocellulose is not yet commercial but it is subject of numerous R&D projects especially in the U.S. It is a promising technology as shown by detailed techno-economic studies by NREL (Aden at al. 2002). Technological breakthroughs in the area of pretreatment of lignocellulose are seen as a key prerequisite to the development of a future bio-based chemical industry.

The BREWtool data belonging to this subsystem can be found in Appendix A1.1 and A1.2.

- The subsystem **"Extraction and processing of non-renewable energy" (No.2)** concerns, in particular, oil and gas. Coal and nuclear energy are relatively unimportant for the processes and sectors taken into account in BREWtool. Apart from being used as feedstock for petrochemicals, non-renewable energy is also converted to steam, power and other utilities which are required for producing both petrochemicals and WB products. The BREWtool data belonging to this subsystem can be found in Appendix A1.2 and in Appendix A2 and A3.

- The subsystem **"Bioprocess" (No.3)** represents the biotechnological conversion of bio-based feedstock to organic chemicals. This subsystem is the core of interest of the BREW project. It is modelled either by use of proprietary data or by application of the Generic Approach (see Section 3.1). The main sections in this subsystem are the seed train, fermentation/bioprocess, filtration and product workup. Relevant data belonging to this subsystem can be found in Appendix A1.2 and Appendix 8 to 10.

- The **subsystem "Management of process waste" (No.4)** concerns, in particular, the treatment of solid biomass and of wastewater originating from the fermentation step. These processes are included in the process flow diagrams developed for the Generic Approach (Section 3.1). It is assumed there all solid biomass waste generated within the production process is incinerated with energy recovery and all waste water is treated on-site by a standard process similar to municipal waste water treatment, with energy requirements being a function of the chemical oxygen demand (COD) of the water. The BREWtool data are given in Appendix A5 (A5-1 and A5-2). For energy recovery with excess power or steam production, the methodology will be explained in Section 3.2.4 and 3.2.5.

- The subsystem **"Management of post-consumer waste" (No.5)** is modelled by assuming transportation and treatment by one of the three options given in Box 3-1. Credits are introduced (both in the environmental and the economic analysis) in order to account for the avoided production of heat and power (as outlined in Section 3.2.4 and 3.2.5; see also Appendix A1.2).

In all subsystems, environmental impacts are caused not only by the *direct* inputs in the form of raw materials, auxiliaries and energy. There are also *indirect* environmental which are related to the production of the capital goods needed. These indirect environmental impacts

related to capital goods are not taken into account in BREWtool because they are known to be of subordinate importance for the production of energy-intensive bulk products as studied in this project (Boustead 2003).

1.) Agriculture/forestry, biomass pretreatment and conversion
- Fermentable sugar (sucrose) from sugar cane
- Fermentable sugar (glucose) from maize kernels
- Fermentable sugar (C_5/C_6 sugars) from lignocellulose (e.g., from maize stover)

2.) Extraction and processing of non-renewable energy
- Extraction
- Transport (seaborne and pipelines for oil; pipelines and domestic for gas; seaborne and pipelines for oil)
- Treatment (refining of oil; relatively simple purification of natural gas)
- Transportation to final user

3.) Bioprocess
- Seed train (production of microorganism)
- Fermentation/bioprocess
- Filtration
- Product workup (several steps)

4.) Management of process waste
- Waste water treatment
- Incineration of biomass waste with energy recovery

5.) Management of post-consumer waste
- Incineration without energy recovery (base case)
- Incineration with energy recovery
- Anaerobic digestion

Box 3-1: Subsystems included in BREWtool

Environmental impact categories

A full-fledged LCA study comprises many environmental interventions,[37] which lead to various environmental impact categories such as the greenhouse effect or acidification. The data representing the size of the environmental interventions are collected in the so-called *inventory table*. To prepare such an inventory table, an LCA typically uses measured data, which is generally most reliable if obtained from an existing plant operating at the scale of interest to the study (for BREW: large-scale plants). In the BREW study, the focus of interest is on future processes for which measured data is not available in many cases. Therefore, a limited number of impact categories have been selected for study in BREW; namely: 1) Non-

[37] *Environmental interventions* represent the flows crossing the system boundaries in an LCA study (see Figure 3-2). Examples are the use of resources (e.g., fossil resources or land) and emissions (e.g., CO_2, NOx and treated wastewater effffluent).

renewable energy use; 2) Renewable energy use; 3) Greenhouse gas (GHG) emissions; and 4) Land use for agriculture. These four impact categories have been chosen reasoning as follows:

- Non-renewable energy is a first proxy of the environmental impact (Huijbrechts et al. 2006) and it represents a straightforward and practical approach because all (industrial) operations require energy. By far the most important component of non-renewable energy is fossil energy, while the share of nuclear energy, which enters the system via grid power, is generally very limited.
- Renewable energy is reported in order to allow an overview of the total energy consumption and hence to provide insight into the overall energy efficiency of the product system studied. Since, in the case of biomass use, renewable energy is indirectly captured by land use we pay limited attention to renewable energy in this report.
- Greenhouse gas (GHG) emissions are of growing importance due to the increasing attention given to the greenhouse effect in policy, companies and by the public. Both fossil carbon dioxide (CO_2) and other greenhouse gases are taken into account in this study.
- Land use for agricultural cultivation will be of increasing importance in the future. With the growth of bio-based energy, bio-based chemicals and land requirements for food production, land use could become the constraining factor and therefore needs to be monitored.

When attempting to interpret results and draw conclusions from these specific impacts it should be kept in mind that for a complete environmental analysis, other impact categories including, for example, water use, acidification, eutrophication, solid waste, particulate emissions, human toxicity and environmental toxicity should also be studied. As such, the scope of the environmental analysis in the BREW is limited to a few key impact categories rather than being a comprehensive environmental assessment in line with full-scale life cycle assessment (LCA) studies.

3.2.2 Methodology for calculating energy use, greenhouse gas (GHG) emisssions and land use

The starting point for the environmental analysis is the mass flows of all inputs (chemicals, fuels, utilities) into the system studied. Inputs to the system include the feedstocks, auxiliaries, (bio)catalysts, fuels and utilities. Each input and output of the product system is characterized by (Figure 3-3):

- its calorific value Y_i (in GJ/t product)
- the cumulative energy use YY_i (from cradle to factory gate) for its production
- its (chemically) embodied carbon X_i
- the cumulative GHG emissions (cradle-to-factory gate) of the inputs XX_i and
- the land use required in the case of bio-based products (not shown in Figure 3-3).

Greenhouse gas (GHG) emissions consist of two components: direct GHG emissions from the product system in the form of CO_2 or CH_4 (as CO_2 equivalents) and indirect releases of greenhouse gases due to the production of the feedstocks and other inputs. These indirect releases include non-CO_2 GHG emissions, in particular nitrous oxide (N_2O) from fertilizer use.

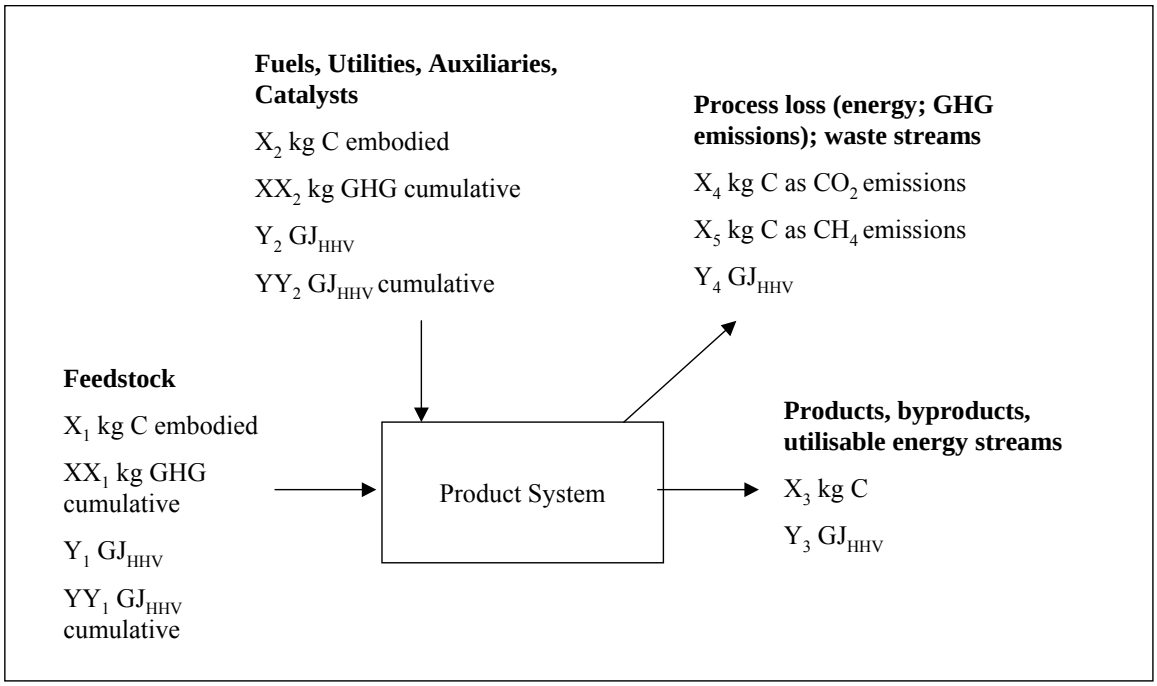

Figure 3-3: Inputs and outputs for the calculation of energy use and GHG emissions in BREWtool

The system carbon balance (equation 1) and the GHG emissions for cradle-to-grave (case: without energy recovery) and cradle-to-factory gate system boundaries (equations 2 to 4) are given below. Cradle-to-grave GHG emissions (base case: no energy recovery – equation 2) are calculated by assuming all carbon inputs leave the system as CO_2 emissions. From this the cradle-to-factory gate GHG emissions are calculated by subtracting the amount of carbon stored in the product (equivalent CO_2 emissions).

Mass balance on carbon

$$X_1 + X_2 = X_3 + X_4 + X_5 \qquad \textit{Equation 1}$$

GHG emissions cradle-to-grave (case no energy recovery)(GHG_{CG})

$$GHG_{CG} = XX_1 + XX_2 + (X_3 + X_4) * f_{CO2} + X_5 * f_{CH4}$$

where f_{CO2} = Conversion factor from carbon to CO_2

f_{CH4} = Conversion factor from CH_4 emissions (expressed in carbon equivalents) to GHG emissions

Rearranging the equation:

$$GHG_{CG} = XX_1 + XX_2 + (X_3 + X_4 + X_5) * f_{CO2} + X_5 * f_{CH4} - X_5 * f_{CO2}$$

Substituting equation 1:

$$GHG_{CG} = XX_1 + XX_2 + (X_1 + X_2) * f_{CO2} + X_5 * f_{CH4} - X_5 * f_{CO2} \qquad \textit{Equation 2}$$

GHG emissions cradle-to-factory gate (GHG_{CF})

$$GHG_{CF} = GHG_{CG} - X_3 * f_{CO2} \qquad \textit{Equation 3}$$

To account for cases for cradle-to-grave systems in which energy is recovered from the product in a post-consumer waste management facility, a credit is introduced and equation 2 modified to give equation 4.

GHG emissions cradle-to-grave (GHG_{CG}) with post-consumer energy recovery

$$= GHG_{CG} - \eta * X_3 * f_{CO2} \qquad \textit{Equation 4}$$

η = efficiency of energy export from the product (post-consumer) in a waste management facility.

$\varepsilon = 0$: zero energy exported; $\eta = 1$: energy equivalent to HHV of product exported.

According to the carbon balance, any output not designated a product, by-product or utilisable energy stream (refer to Figure 3-3) is defined as a waste stream. All carbon leaving as waste streams is assumed to enter the atmosphere rather than to be fixed in solid or liquid form. As a default, carbon losses are assumed to occur in the form of CO_2 but corrections are made for methane wherever relevant. Carbon released to the atmosphere and originating from biomass is considered *not* to contribute to the greenhouse effect, which, in contrast, is the case for carbon of fossil origin.

All energy flows are expressed in terms higher heating value (HHV). The system energy balance and the energy use for cradle-to-factory gate and cradle-to-grave system boundaries are given in equations 5 to 8 below.

Energy balance

$$Y_1 + Y_2 = Y_3 + Y_4 \qquad \textit{Equation 5}$$

Primary energy use cradle-to-factory gate (E_{CF})

$$E_{CF} = YY_1 + YY_2 \qquad \textit{Equation 6}$$

Primary energy use cradle-to-grave (E_{CG}) without energy recovery

$$E_{CG} = E_{CF} \qquad \textit{Equation 7}$$

Without energy recovery, cradle-to-grave energy use is identical to cradle-to-factory gate energy use because energy consumption in transport of the used product to waste treatment and in the management facility itself can be assumed to be negligible.

As in the case of the carbon balance, credits are used to account for cases in which energy is recovered from the product in a post-consumer waste management facility (equation 8).

Primary energy use cradle-to-grave (E_{CG}) with post-consumer energy recovery

$$E_{CG} = E_{CF} - \eta * Y_3 \qquad \textit{Equation 8}$$

Calculation of land use is based on long-term average crop yields (tonnes per hectare, t/ha) for the crop in the specified geographical region.

3.2.3 Co-product allocation (partitioning)

In several production systems modeled in this study, co-products are produced. Inputs and outputs to the system thus have to be allocated (i.e. assigned via a partitioning parameter) to both the main product and co-products. A number of allocation methods are used in BREW, namely:

1) If the main product and the co-product are of similar economic value and if *no* detailed information is available for the co-product (cradle-to-factory gate energy and emissions),

partitioning of inputs and outputs between the main product and the co-product is conducted on a product **mass** basis.

2) If the main product and the co-product are of similar economic value and if detailed information *is* available for the co-product, the inputs and outputs are *not* partitioned, but instead **credits** are given for the co-product. The credits represent the impact for an alternative process route leading to the co-product *only*.
3) The cases above refer to situations where the main product and the co-product do not differ decisively in economic value (price). For cases in which the difference in economic value is substantial (around a factor of 2 or more), partitioning is performed on a product **price** basis. This means that a higher share of the overall environmental impacts is assigned to the high value products than in the case of mass-based allocation. For example, price-based allocation has been used for glycerol as a by-product of biodiesel production.
4) When energy is generated from a waste material generated in the process, this is accounted for by means of credits. For example, this is the case for the lignin-rich waste stream produced in a maize stover hydrolysis process. The lignin is fed to an on-site waste-to-energy facility and of the steam and electricity thus generated, a proportion is used in the hydrolysis process, with the remainder being exported from the process boundary. The waste-derived energy used on-site reduces non-renewable energy requirements for the process, while for exported energy, an equivalent amount of avoided non-renewable energy (in primary terms) is allocated to the process. The methodology is explained in more detail in the next section.

3.2.4 Methodology for calculating energy and emission credits for exported energy

When electricity or steam is exported for use outside the system boundary, energy credits are assigned to the system. If only non-renewable energy is used in the product system, then it is rather obvious to deduct the credit from the input in order to determine the net non-renewable energy use (NREU). If, however, the exported energy originates from renewable energy sources then a choice may be made whether to deduct the credits from the input of renewable energy, of non-renewable energy or to a share of both. According to the methodology implemented in BREWtool the credit is always deducted from the inputs of non-renewable energy as shown in Figure 3-4. The reasoning behind this methodology is that non-renewable energy is dominating in the current energy system (in all sectors of the economy) and that this will continue to be the case also for the next decades. It is therefore justified to consider credits (from renewable energy) to replace non-renewable energy. For reasons of consistency, we apply this methodology to the entire time period studied even though the importance of renewable energy might increase substantially in the decades to come (this depends primarily on developments outside the chemical sector and is therefore beyond the scope of ananlysis of this study).

When a renewable feedstock input to the system results in a renewable energy output from the system, this renewable energy output is credited with an avoided amount of non-renewable energy as follows:

- **Steam**: primary equivalent of steam based on the partial fuel utilization efficiency for medium pressure steam production in the EU-15 chemical industry of 76.9% = 1.3 GJ primary energy/GJ steam (for details see Appendix A2; in particular Table A 2.5);
- **Electricity**: weighted average conversion factor for electricity used in the EU-15 Chemical Industry of 39.6% = 2.5 GJ primary energy/GJ electricity. Appendix A2 gives

full details of the calculation of these two conversion factors (for details see Appendix A2; in particular Table A 2.4).

All data related to power generation and heat raising refer to the base year (2000); i.e. for both present and future scenarios we assume production of steam and electricity according to the conversion factors for 2000. The reason for this assumption is that our focus of interest in this study is on the contribution of White Biotechnology to more efficient and economically more viable production routes in the chemical sector. We decide *not* to superimpose these results with the effect of changes in power generation and steam production because very diverse effects can be expected depending on whether, for example, the power system shifts primarily to coal or to nuclear energy.

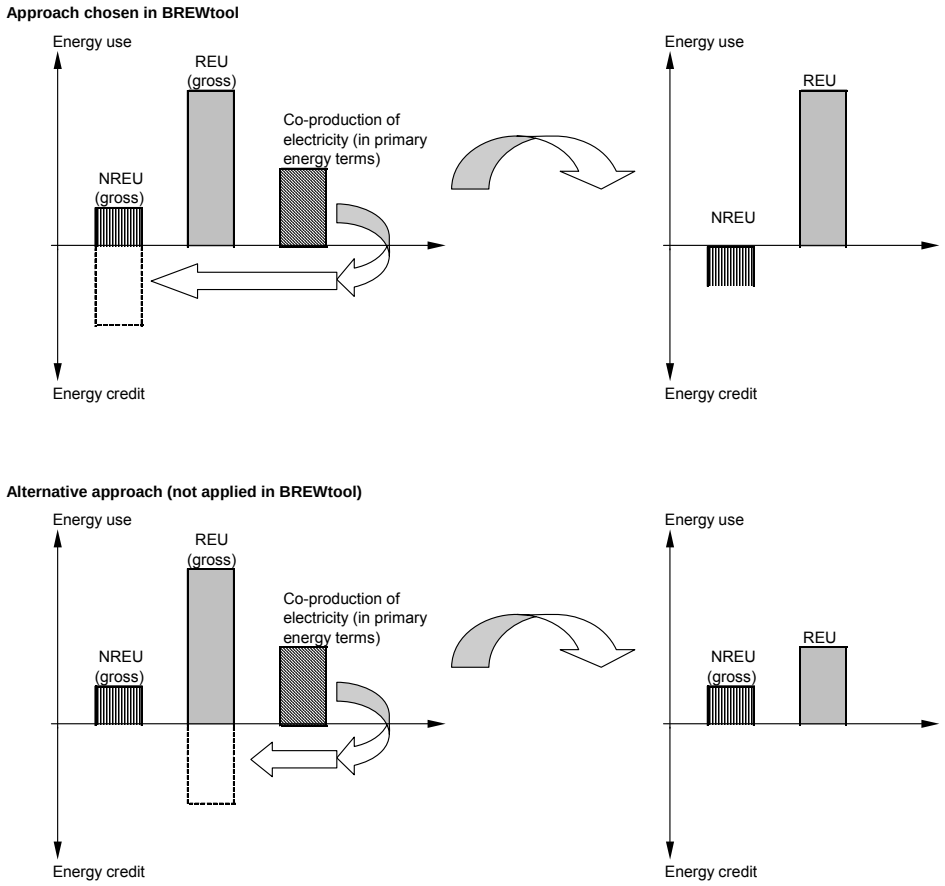

Figure 3-4: Methodology for giving credits for exported energy

3.2.5 Management of combustible waste

Bio-based chemicals may lead to considerable amounts of combustible waste. If the waste is generated as part of the production process it is referred to as *pre-consumer waste*. Once the organic chemicals have reached the end of their useful life *post-consumer waste* is generated; this waste is also combustible (or rather: the final products they are used for).

In White Biotechnology processes, substantial amounts of biomass waste become available from the fermentation process. We assume this *pre-consumer waste* to be incinerated with energy recovery for steam and power generation (see Appendix A5-2).

Likewise, *post-consumer waste* originating from organic chemicals can also be incinerated. This may occur with or without energy recovery. Organic chemicals – regardless of whether they are of petrochemical or of bio-based origin - can be used to manufacture *biodegradable* materials, which ultimately becomes biodegradable post-consumer waste. It should be noted that bio-based chemicals are not necessarily biodegradable; in order to avoid biodegradability they are usually subjected to one or more conventional chemical process which may involve petrochemical reagents. Apart from incineration, biodegradable waste can be treated by anaerobic digestion or by composting.

Depending on the type of the waste stream and the further progress of technology it may be possible to use it as raw material instead of disposing of it (usually by incineration). Lignin is a widely named as possible future candidate as chemical feedstock (e.g., Ribbons 1987) but, to date, R&D has failed to identify attractive large-scale uses as raw material. Finally, landfilling is, in principle, a waste management option for all types of waste.

Actually the organic chemicals do not reach the waste management stage as such but they are embedded in final products, which are disposed of (e.g., the carpet of a car made from polytrimethylene terephthalate, PTT; PTT is made from the alcohol 1,3-propanediol which can be produced by means of White Biotechnology). Nevertheless we calculate in BREWtool, the environmental impacts of the waste treatment of the *pure* components (PTT; 1,3-propanediol) in order to understand the importance of this stage in the process chain.

Landfilling is excluded from the calculations performed in the BREW project because landfilling of synthetic organic materials is prohibited in many European countries. Waste incineration both with and without energy recovery is included in BREWtool because these waste management methods are universally applicable for all types of combustible waste. Waste incineration with energy recovery leads to energy byproducts in the form of steam, low temperature heat and/or electricity, which need to be accounted for in the environmental assessment. Waste incineration with energy recovery is therefore discussed below. Anaerobic digestion also leads to energy credits, which is therefore also included in BREWtool and is discussed below. In contrast, composting was excluded from the BREW project as potential waste management option: The composting process yields compost, which is a valuable product for horticulture, gardening and also for agriculture depending on soil/erosion conditions. However, the overall environmental benefits are difficult to quantify; for energy and greenhouse gasses – i.e., the environmental impacts covered by BREWtool – the benefits seem rather small. Deactivation of the compost, which may become a necessity due to the use of genetically modified organisms in fermentation, may even overcompensate the benefits. For these reasons, composting was excluded from the BREWtool calculations.

Incineration of post-consumer waste with energy recovery takes place primarily in waste-to-energy facilities, which are mostly municipal solid waste incineration plants, MSWI (Phylipsen et al. 2002). The efficiencies of these waste-to-energy facilities differ decisively: While, in many cases the electricity and/or steam produced represents only a few per cent up to 10% of the heating value of the waste input, efficiencies of 70% and more have been realised in exceptional cases. It has been assumed in this study that the average output of all incineration facilities (both simple incineration and waste-to-energy facilities) is 12% heat and 12% electricity (relative to the HHV of the waste input; Patel 1999). Figure 3-5 shows the

energy flows and avoided primary energy (credits to non-renewable energy) for waste-to-energy incineration as used in BREW calculations. **Anaerobic digestion** (also exclusively assumed for post-consumer waste) leads to the production of biogas, which is used to generate steam/electricity for export. Figure 3-6 shows the energy flows and avoided primary energy (credits to non-renewable energy) for anaerobic digestion as used in BREW calculations. More detailed calculations for this option are given in Appendix A5-3.

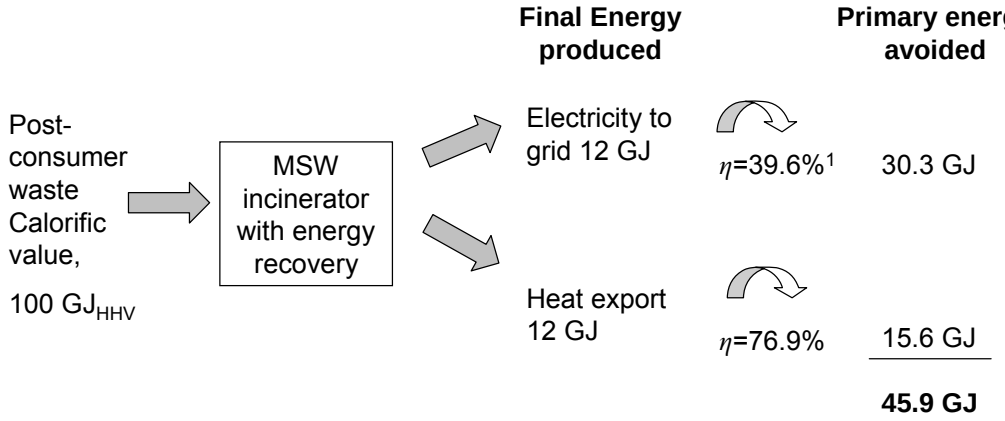

Figure 3-5: Energy credits from incineration of post-consumer waste

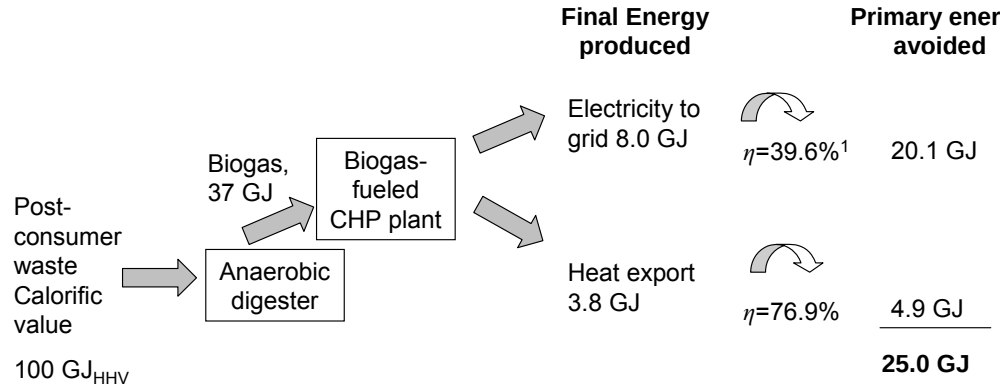

Figure 3-6: Energy credits from anaerobic digestion of post-consumer waste

3.3 Methodology of the economic assessment

Quantitative assessments of the economics of bio-based bulk chemicals produced by White Biotechnology are even scarcer in the public domain than environmental assessments. As for environmental assessments, the few analyses on economics lack consistency in terms of basic data and key assumptions. Therefore, BREWtool has been designed to include also an economic evaluation tool.

3.3.1 Methodology for economic assessment

The economic assessment implemented in BREWtool is in line with standard business economics. As shown in Figure 3-7, the calculation is performed according to the following steps: firstly, variable costs (feedstocks, auxiliaries/catalysts, by-products, utilities,[38] waste treatment) and fixed costs (supplies, labour) are added to obtain the total direct operating cost; then taxes, insurance fees and plant overhead are added to this figure and also an allowance for marketing, administration and R&D is added to give the production costs without depreciation,[39] finally, the so-called *capital charge* is added which is calculated by multiplying the *total fixed capital* (TFC; identical with total investment) with a fixed percentage. The capital charge represents the total of both *depreciation and profits*. In consultation with the BREW industry partners a percentage of 30% was used to calculate the capital charge (see Figure 3-7). By adding the capital charge to the production costs without depreciation, the *product value* is determined which is also referred to as *profited production cost*. The product value is the total of production costs plus profit and it represents an approximation of the *market price*. The real market price may be higher or lower than the product value depending on demand and supply (e.g., depending on whether there is harsh competition or an oligopoly, whether production facilities are depreciated or not etc.; see also discussion in Section 3.4.4).

The economic analysis in BREWtool refers exclusively to the *production* of one mass unit of the chemical studied (e.g., 1 tonne of polylactic acid), while the use phase and the waste management stage are excluded. The economic analysis hence refers to the system "cradle-to-factory gate" and not to the system "cradle-to-grave". The extension of the economic analysis to "cradle-to-grave" is done in so-called *Life Cycle Costing* (Rebitzer and Seuring 2003) which, however, is generally only useful if performed for final products (e.g., the bumper of a car).

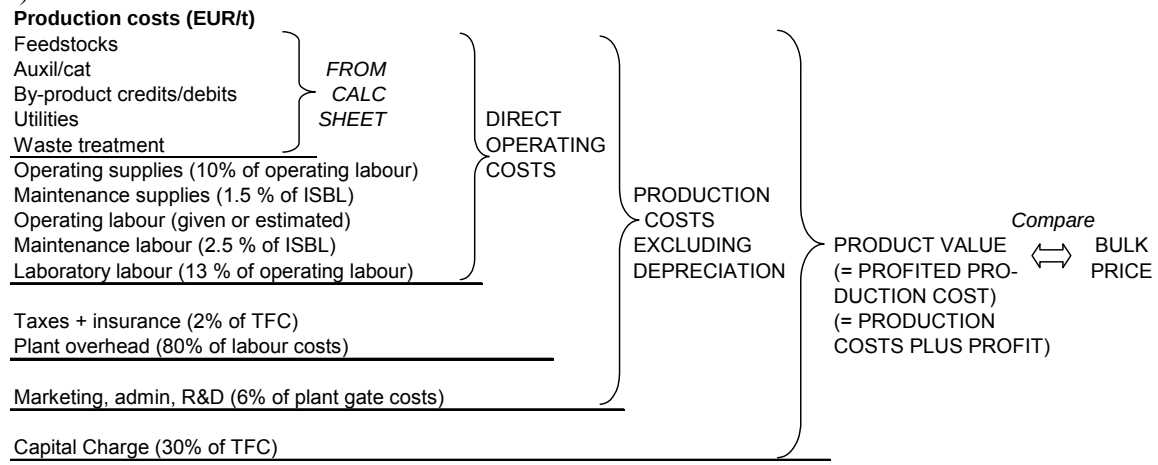

Figure 3-7: Methodology for calculating the product value

According to the calculation methodology (Figure 3-7), certain costs are assumed to be related to capital investment, e.g. maintenance supplies and maintenance labour are proportional to the *inside battery limits* (ISBL) investment; taxes and insurance are proportional to the *total fixed capital* (TFC). *Inside battery limits* refers to the process

[38] (Variable) costs for utilities do NOT include capital charges as these are accounted for in the outside battery limits (OSBL) capital investment costs.
[39] Depreciation is instead included in the Capital Charge (see below).

equipment, including feed treatment, (bio-)chemical conversion, product separation and purification, recycle handling and product packaging. *Outside battery limits* (OSBL), also know as "*offsites*", designates all investments which are not specific to the process but are nevertheless required by the process; main items are bulk storage, utilities and service facilities. The costs of utility generating services, i.e. steam boilers, water treatment units, cooling towers, refrigeration units, etc. are also included in the OSBL costs. The total fixed capital (TFC) is the sum of ISBL and OSBL. Capital investment is annualised (in € per tonne per annum).

The calculation of product values has been performed for all bio-based chemicals studied (see Table 3-1, 21 products, 95 process routes). The calculation procedure for product values has also been performed for the key petrochemical products which were chosen as reference. The application of the methodology according to Figure 3-7 implies that *also for all inputs* (especially feedstocks and auxiliaries) product values (*not:* prices) are used. We have followed this principle as far as possible and reasonable: For example, the product values are used for the feedstock (e.g., for ethylene or ethanol used as raw material) if it is a major cost component and if it is subject to change (e.g., as will be discussed in Chapter 4, the values can differ decisively depending on the scenario assumptions). We depart from this principle for raw materials upstream in the process chain (e.g., for naphtha or for fermentable sugar; see Section 4.4) where we either apply simplified relationships (e.g., for naphtha) or exogeneously set the values (e.g., for fermentable sugar). We also use prices (instead of product values) and simple assumptions about their future development for inputs that are used in small quantities (especially auxiliaries and catalysts).

3.3.2 Scale-up

To allow for processes of different design capacity to be compared to one another, capital investment figures of bio-based processes have been scaled to a capacity of 100 kt p.a. according to the following equation:

$$I_2=I_1*(C_2/C_1)^{f\_cap} \qquad \textit{Equation 9}$$

where C_1 is the original capacity; C_2 is the new capacity; I_1 is the original capital expenditure; I_2 is the new capital expenditure; and f_cap is the scaling exponent. f _cap= 0.7

An additional consideration in scale-up is the operating labour requirements. In consultation with the industry partners, the following equation has been used to account for operating labour requirements in scale-up situations:

$$L_2=L_1*(C_2/C_1)^{f\_lab} \qquad \textit{Equation 10}$$

where C_1 is the original capacity; C_2 is the new capacity; L_1 is the original labour requirement; L_2 is the new labour requirement; and f_lab is the scaling exponent. f _lab= 0.25

A scaling exponent of f _lab= 0.25 has been used.

The scaling factors both for labour and for capital were used for all bio-based processes except for the Generic Approach, for which. Scaling was, in particular performed for proprietary data received from the partners, for SRI data and and for data from the open literature. Scaling was not necessary for the Generic Approach because a scale of 100 kt was chosen from the outset and larger sizes were assumed for the sensitivity analyses (see Table

3-2). The investment costs for the Generic Approach were calculated by DSM by use of their so-called *Functional Unit Method* (*FUM;* DSM, internal document).

3.3.3 Interpreting the results

In order to put the results of the economic analysis of bio-based products into perspective and in order to interpret them we proceed as follows:

i) **Under present-day market conditions** we use primarily the product values of the petrochemical equivalents as benchmark for the results for bio-based chemicals; however, we compare the results for bio-based chemicals also to current market prices (Section 3.4.4).
ii) **Under future market conditions** (scenario analyses) we exclusively use *product values* as benchmark and calculate the product values of the petrochemical equivalents according to the methodology explained above.

The economic assessment of future processes is unavoidably subject to substantial uncertainties. We estimate that, in exceptional cases, the error may be as high as ±50%, especially due to assumptions made about future technical performance. However, the comparison for current technology under present-day market conditions shows much smaller uncertainties and demonstrates that, exceptions excluded, the method implemented and the data used are valid also for the future.

The results for currently prevailing conditions are discussed in Chapter 3.4 (for 21 products) while the analysis for the future dealt with in Chapter 4 (Scenario projections).

3.4 Results of the environmental and economic assessment per product

For the remainder of Chapter 3, we compare the bio-based production by means of White Biotechnology according to the *current and the anticipated future* state of the art with the production of petrochemical equivalents according to the *current* state of the art. The comparison is performed for the functional unit of one tonne of organic chemical. The energy prices assumed for this comparison on a *product-by-product basis* are representative for the end 1990s/first few years of the 21st century (US$ 25/barrel crude oil and 4 €/GJ for natural gas for final users in the chemical sector; Appendix A3-2). We use these energy prices to assess both processes based on current and future technology. The results presented in this chapter lay the foundation for Chapter 4 in which scenario projections for White Biotechnology products are developed. In addition to the results presented in this Section 3.4, the scenario projections in Chapter 4 account for the impact of higher fossil fuel prices on the economics of both petrochemical and bio-based chemicals. Moreover, while the comparisons made in this section (Section 3.4) are based on the functional unit of one tonne of product, the projections in Chapter 4 account for the difference in market potentials across the products studied (for example, the market potential of adipic acid is expected to be much lower than for polylactic acid or ethanol for chemical purposes).

As some of the data provided by the partners are confidential, all results are presented in this chapter in aggregated form: for the environmental assessment, the results presented refer to the entire process chain from cradle-to-factory gate and, alternatively, to the system cradle-to-grave. For the economic assessment, the results presented refer to the system cradle-to-factory gate, which is in line with standard business economics.

This subchapter is structured as follows: In Section 3.4.1 we study the environmental impacts of producing fermentable sugars from various feedstocks and we present our assumptions regarding the economics of fermentable sugars. Section 3.4.2 reports the results of the techno-economic analysis of 1,3-propanediol (PDO) as exemplary case for a White Biotechnology product made by fermentation. Section 3.4.3 and 3.4.4 provide, in condensed form, the results of the environmental and the economic analysis for all fermentation-based products studied. Section 3.4.5 presents the results for four enzymatically produced products; these products are considered to be representative for enzymatic conversions, hence allowing to draw first general conclusions (Section 3.4.5).

3.4.1 Fermentable sugar

For the environmental assessment of all White Biotechnology products produced by fermentation, three types of fermentable sugars have been assumed. These are dextrose from maize starch, sucrose from sugar cane and mixed sugars (C_5/C_6) from maize stover. In addition, glycerol and vegetable oil was studied as

fermentation feedstock but we will not discuss these feedstocks in this section because they were only assumed for very few process routes.[40]

The three types of fermentable sugar are assumed to be interchangeable as feedstock (1 t dextrose = 1 t sucrose = 1 t maize stover sugars), implying that the yield on each biotechnological process studied is independent of the type of sugar feedstock. This is not strictly true since the microorganisms involved in the biotechnological conversion of sugar feedstock to the desired chemical are engineered for a specific feedstock (e.g., dextrose). If a different feedstock is used the yield may change, as may the impurity profile and downstream processing characteristics. In this study we assume that such differences can be overcome by R&D and are therefore negligible for the assessment of future processes (compare Section 3.1.1).

In this section, key features of the processes for the production of fermentable sugar are described and some explanations are given on the cradle-to-factory gate environmental impacts of the fermentable sugars as shown in Table 3-5. The environmental analysis is then summarized before presenting the approach chosen for the economic analysis.

[40] Vegetable oil is directly used only for few processes covered in the BREW study:

- Firstly, it is used for three of the processes leading to polyhydroxyalkanoates (PHA), namely for i.) BioPHAmcl-A&F-FA-Oilex, ii.) BioPHA-GA-OilTexey and iii.) BioPHAmcl-A&F-D5:FA1-Tex, where a glucose:oil = 5:1 mixture serves as feedstock).
- Secondly, glycerol (which is produced as by-product from splitting of vegetable oil) is used as feedstock for the production of PDO in two processes, i.e. i) PTT-bioPDO-Anaer-Glyc-SRI-Td and ii) PTT-bioPDO-Anaer-Glyc-VDI-Td. Information on the effects of different ways of allocation between the main product and glycerol and the consequences for the final results are given in Section 3.4.2.
- Finally, most of the products discussed in Section 3.4.5 (Energy analysis and techno-economic assessment for enzymatic conversions) originate from vegetable oils. Since, however, the same is true for the respective conventional processes used as benchmark for the comparison, the environmental impacts related to the supply of vegetable oils cancel out and therefore do not need to be studied.

All data per tonne of fermentable sugar		1 Total renewable energy REU GJ_{HHV}/t	2 Process energy NREU GJ_{HHV}/t	3 Exported energy = NREU credits GJ_{HHV}/t	4 (=2-3) NREU GJ_{HHV}/t	Ran-king	NRGHG emissions t CO_2 eq./t	Ran-king	Seques-tered CO_2 t CO_2/t	NRGHG minus sequestered CO_2 t CO_2 eq./t	Land use ha/t	Ran-king
Dextrose (32%ds) from starch (maize, wet milling)[1]	A. Default (Detailed mass-based allocation)	17.3	6.2	0.0	6.2	6th	0.40	6th	1.47	-1.07	0.13	3rd
	B. Sensitivity (High energy use for maize)	17.3	10.3	0.0	10.3	7th	0.63	7th	1.47	-0.84	0.13	3rd
Sucrose (59%ds) from sugar cane [2)-6)]	C. Default (Energy credit approach)	41.8	1.7	14.5	-12.8	1st	-0.54	1st	1.54	-2.08	0.13	3rd
	D. Sensitivity (Economic allocation, 20%)	33.4	1.4	--	1.4	5th	0.11	4th	1.54	-1.43	0.10	2nd
C5/C6 sugars (13%ds) from lignocellulosics [7]	E. Default (maize stover, econ. alloc.)	29.2	4.9	9.2	-4.4	2nd	-0.16	2nd	1.46	-1.62	0.05	1st
	F. Sensitivity (poplar)	35.6	7.6	9.2	-1.7	4th	0.14	5th	1.46	-1.32	0.26	4th
	G. Sensitivity (miscanthus)	34.3	5.2	9.2	-4.0	3rd	-0.04	3rd	1.46	-1.50	0.13	3rd

NR: Non-renewables-sourced; R: Renewables-sourced

1) Vink, E.T.H., Hettenhaus, J., O'Connor, R.P., Dale, B.E., Tsobanakis, P., Stover, D.: (forthcoming a): The Life Cycle of NatureworksTM Polylactide. 2. The production of dextrose via corn wet milling. Cargill Dow BV, Naarden. Aug 16.

2) Sugar cane in Brazil, UU calculations. Average of 2 cases to account for differences in sugar cane composition (Case 1: high sucrose content; Case 2: medium sucrose content).

3) Carvalho Macedo, Isaias De (1992): The sugar cane agro-industry -- Its contribution to reducing CO2 emissions in Brazil, Biomass and Bioenergy, Volume 3, Issue 2, pp77-78.

4) Carvalho Macedo, Isaias De (1997), Greenhouse gas emissions and avoided emissions in the production and utilization of sugar cane, sugar and ethanol in Brazil:1990-1994, Report for MCT - Coordenacao de Pesquisa em Mudancas Globais, pp5-6.

5) Damen, K. (2001): Future prospects for biofuel production in Brazil, M.Sc. report, Department of Science, Technology and Society, Utrecht University, Utrecht, Netherlands, November 2001

6) Braunbeck, O., Cortez, L., Walter, A. (1999): Sugar cane resources for sustainable development: A case study in Luena (Zambia). Report for the Stockholm Environment Institute, February, p.11.

7) Calculated in BREWtool with NREL data for 2010 design case (Aden et al., 2002), assuming 34% of on-site energy production allocated to pretreatment + hydrolysis.

Table 3-5: Overview of energy and emission data for sugar feedstocks as used in the BREW model calculations (system boundary: cradle to fermentable sugar)

Fermentable sugar from maize

Dextrose ($C_6H_{12}O_6$) is produced from starch crops such as maize or wheat, which both grow in moderate climate. Starch is converted into dextrose using enzymes for starch liquefaction and hydrolysis with a yield of 95%, producing 0.64 kg dextrose/kg dry maize (dry solids; this translates to a gross dry maize input of 1.0/0.64 = 1.56 t maize/t dextrose). Other products apart from starch are germ, maize gluten feed, maize gluten meal and heavy steepwater. For maized-derived starch, we base our model calculations largely on NatureWork's publication titled "The production of dextrose via corn wet milling" (Vink et al., forthcoming a), which contains results for three allocation approaches:

1.) The detailed mass-based allocation according to Vink et al. (forthcoming a) is used as default dataset in BREWtool (see row A in Table3-5). Vink et al. (forthcoming a) study the mass balances for each subprocess separately and account for the fact that some products require only one or two processing steps while others (in particular dextrose) run through all processing steps. While the gross maize input per kg of dextrose is 1.56 kg maize (see above), the net input after accounting for all byproducts is 1.06 kg (Vink et al., forthcoming a). For agricultural production, the environmental impacts have been allocated to maize versus maize stover using the respective prices (for maize stover only the share removed from the field has been taken into account, i.e. 13%; the assumed maize stover price is 30 $/ton and the maize price is118 $/ton; Vink et al., forthcoming b). The default data and also the datasets No. 3 and No. 4 (see below)

represent the situation in the U.S. which is known for its large-scale and low-priced maize. Given the favourable conditions for maize cultivation in the U.S., the environmental impacts according to the default dataset in BREWtool may be somewhat underestimated for Europe.

2.) For this reason, higher values for non-renewable energy use have been assumed for maize production (5.47 GJ/t) in the sensitivity case (see row B in Table 3-5). The higher values originate from Boustead and Panvalkar 2001) and may hence be more representative for the production in Europe.

3.) The simple mass-based allocation (perfomed by Vink et al., forthcoming a) differs from the sophisticated mass-based allocation (as applied in No. 1 and No. 2) by not taking subprocesses into account. The overall environmental impacts are allocated to the individual products on the basis of the mass of the final outputs. The data resulting from this approach are not taken into account in BREWtool.

4.) In the economic allocation, Vink et al. (forthcoming a) allocate the overall environmental impacts to the individual products on the basis of the economic values of the final outputs. The data resulting from this approach are neither included in the BREWtool calculations.

The results for non-renewable energy use according the default allocation method in BREW are rather close to those of allocation method No. 3 and No. 4 (up to 20% difference) and nearly 40% lower than according to method No. 2. The results for greenhouse gas emissions are even practically identical for the allocation methods No.1 (default), No. 3 and No. 4: In these three cases the GHG emissions (without deduction of the sequestered amounts) are around 0.4 kg CO_2 eq./kg product, which is approximately around 60% lower than method No. 2. The results calculated with the approaches No. 1 and 2 (row A and B in Table 3-5) hence cover the entire range of results that would be obtained by applying all four approaches.

Fermentable sugar from sugar cane

Sucrose ($C_{12}H_{22}O_{11}$) is produced by milling of sugar cane. Sugar cane only grows in tropical climate and therefore does not represent an indigenous feedstock source for Europe. Bagasse, i.e. the leftovers from the milling process, is burnt to generate energy. Several allocation procedures are possible for this process. The most plausible approach may be to choose the total factory input of sugar cane as starting point and to assign credits to the process for the exported power. This energy credit approach has been chosen as default for all BREWtool calculations using sugar cane (see Table 3-5, row C; note that the allocation has not been applied to land use which represent total requirements[41]). Alternative approaches are the allocation on mass basis and economic allocation. If allocation is performed on a mass basis, between two thirds and three quarters of the overall environmental impacts are allocated to bagasse, while a relatively low share of the overall impacts is allocated to sucrose. Since bagasse is a low-value product with limited possibilities for use, we do not consider this allocation procedure to be an adequate solution. We therefore conduct an economic allocation. If only the costs for handling and transporting the bagasse is taken into account, then only a few percent (1-3%) of the overall environmental burden are allocated to bagasse. Higher allocation ratios of 10-20% are found if bagasse is assumed to be used as animal feed. In a full-fledged bio-based economy waste flows such as bagasse would be used for energy purposes and/or as chemical feedstocks and would be traded at clearly higher prices than in case of use as animal feed.

[41] It is not straightforward to devise an allocation method for land use. An option could be to allocate land use on the basis of the prices of sucrose versus power/heat.

For our sensitivity calculations (see Table 3-5, row D) we assume that bagasse becomes a desired animal feed and therefore assign 20% of the overall environmental burden to bagasse while the remainder is allocated to sucrose. The comparison of this 20%-economic-allocation with the results according to the default data (row C in Table 3-5) yields the following picture: In the allocated approach (sensitivity; row D), the

- non-renewable energy use (NREU) is higher by 1.4 – (-12.8) = 14.2 GJ/t
- renewable energy use (REU) is lower by 41.8 – 33.4 = 8.4 GJ/t

Both the non-renewable energy use and the overall energy use (total of NREU and REU) are hence clearly higher (by 5.8 GJ/t) in the 20%-economic-allocation compared to the default dataset for sucrose according to Table 3-5. The reason is that the avoided environmental impacts are much larger if bagasse is used to produce energy compared to its use as animal feed.

Fermentable sugar from lignocellulosics

Fermentable sugars from lignocellulosics such as woody biomass are considered a key component of a bio-based economy because they are foreseen to provide fermentation feedstocks at low price also in moderate climate due to the wide availability of lignocellulosic biomass in the form of agricultural waste (e.g., maize stover). The process, which is also referred to as "pretreatment" is not yet commercially available (Cherry and Wenger 2005). The conversion from lignocellulosics to fermentable sugar involves cleaning and chipping of the biomass, hydrolysis of the hemicellulose (physical, chemical or biological), hydrolysis of the cellulose (acid or enzymatic hydrolysis) and post-treatment (Hamelinck 2004). Depending on the process, such pretreatment units may generate large amounts of energy from the lignin and other compounds contained in the biomass. Fermentable sugars from woody biomass are typically a combination of dextrose, xylose and smaller quantities of other sugars. The mixture of sugars is often referred to as C_5/C_6 sugars. There are numerous large research projects especially in the U.S., which aim to convert maize stover (i.e., the stalks and leaves of the maize plant) into fermentable sugars. Maize stover has therefore been chosen as default case in the BREW study. The data shown in Table 3-5 (row E to G) are based on the most detailed, publicly available study on the topic, which was prepared by Aden et al. (2002) at NREL. The study by Aden et al. only provides information for the conversion from maize stover to lignocellulosics. For the purpose of the BREW study, the preceding supply chain providing maize stover and other lignocellulosic raw materials needs to be added; this ultimately leads to the datasets in the row E to F of Table 3-5.

In order to develop the dataset for maize stover (row E), another allocation issue must be resolved: In mass terms, maize kernels and maize stover represent similar shares of the maize plant. Since the main purpose of the cultivation of maize has been and will continue to be the production of starch from the maize kernels it is not reasonable to assume mass allocation between kernels and stover. We have therefore chosen economic allocation as do Vink et al. (forthcoming b ; NatureWorks), thereby assuming prices of 118 US$/ton for corn and 30US$/ton for corn stover (NatureWorks, pers. comm., 2005). The resulting data for maize stover is shown in Table 3-6 (Note: the data in Table 3-6 refer to maize stover and other lignocellulosic feedstocks as such; they do not refer to fermentable sugars as does Table 3-5). As the table shows the energy use and GHG emissions for maize stover are particularly low. This explains why an ethanol plant operated with maize stover can be a net producer of energy (see Table 3-5); since product separation and purification of the ethanol is rather

energy intensive this is only possible by co-production of considerable amounts of excess energy in the pretreatment stage (as represented by the negative values in row E).[42]

In the case of a bio-based economy, the amounts of lignocellulosics available from agricultural waste streams may not be sufficient to cover the total demand. The cultivation of short rotation woody biomass such as poplar or miscanthus may then be the most cost efficient and land efficient solution. As shown in Table 3-6, the energy use, emissions and land requirements are substantially higher for poplar compared to maize stover. As a consequence, the net energy credit for producing fermentable sugars from poplar according to Table 3-5 (row F) is very small and the and there is even a small penalty for GHG emissions (see column "NRGHG emissions"). The energy requirements and GHG emissions for the supply of fermentable sugar from miscanthus (row G) are clearly lower than for poplar and are similar to maize stover except for land use (see Table 3-5).

	Calorific value (heating value) GJ/t	NREU (cradle-to-factory gate) GJ/t	NRGHG (cradle-to-factory gate) t CO_{2eq}/t	Land use CF ha/t
Maize stover	18.1 (only heating value of stover)	0.78	0.07	0.03
Short rotation poplar	19.9	2.29	0.24	0.14
Miscanthus	19.2	0.97	0.14	0.07

Table 3-6: Energy use, greenhouse gas emissions and land use for 1 tonne of maize stover and short rotation poplar

Summary of environmental analysis for fermentable sugars

We consider the energy credit approach for sucrose from sugar cane to be a justified under the assumption of a bio-based economy and therefore base our final conclusions on the default case for sucrose instead of the 20%-economic-allocation. On this basis the results in Table 3-5 can be summarized as follows: Non-renewable energy use (NREU) and non-renewable greenhouse gas emissions (NRGHG) are lowest for sucrose from sugar cane (default approach) and highest for dextrose from maize. The results for C_5/C_6 sugars from lignocellulosics and the results for all other cases lie between these extremes (the ranking is also given in Table 3-5). Regarding land use, it is somewhat more difficult to draw conclusions directly because no allocation was performed for the default case for sucrose (i.e., no land was assigned to the by-production of power; the value in row C of Table 3-5 is hence a gross value). Taking this into account it is, however, safe to conclude that land requirements are lower for sucrose than for starch-derived sugars. For sugars from lignocellulosics, we find a wide range of values: land requirements are particularly low for sugars from corn stover, are similar to maize-derived dextrose in the case of miscanthus and are clearly larger for poplar.[43]

[42] By tracing the material flows in the flowsheets prepared by Aden et al. (2002) it was found that 92 mass-% of the combustibles entering the combustion plant originate from the pretreatment process while only 8% originate from the conversion of the combustible sugars to ethanol.

[43] Land use requirements are in the range of 0.10 to 0.13 ha per tonne with the exception of C_5/C_6 sugars from poplar (0.26 ha/t; see Table 3-5) and from maize stover according to the default case (only 0.05 ha/t). For poplar,

It is of interest to consider the position of sugar cane if sucrose is provided without co-production of power. We can approximate this case by the 20%-economic-allocation for sugar cane (row D), where only a small credit is given to the bagasse. Based on the results of Table 3-5 we conclude that the use of sugar cane without power co-production would lead to energy requirements and GHG emissions which lie between those of corn stover (default; row E) and dextrose from maize (default; row A).

To summarize, we conclude that sugar cane (default; row C) is the most preferable crop for producing fermentable sugar in terms of energy use and GHG emissions and that it outpaces most (if not all) other options also with regard to land use. However, sugar cane cannot be cultivated in Europe. The best option for Europe would therefore be the use of C_5/C_6 sugars from lignocellulosics, if this technology can be successfully commercialized.[44] It must be emphasized that the production of fermentable sugars from lignocellulose is still in the R&D phase and that it is still uncertain whether this technology will ultimately be successful (Cherry and Wenger 2005). Dextrose from maize starch is the least desirable option in terms of non-renewable energy use and greenhouse gas emissions (rank No. 6 and 7) but has the major advantage of being a readily available option for Europe at a large scale. If fermentable sugar from lignocellulosics turns out *not* to be technologically or economically viable in Europe, then starch-based fermentable sugar is the only option for Europe.
If, on the other hand, the conversion of lignocellulosics to fermentable sugars will succeed, the use of maize stover would be most preferable, followed by miscanthus and finally, poplar. Numerous other crops and types of waste should be considered in addition to the few raw materials studied here. Designated crops like miscantus and poplar will most likely be required in large quantities in a full-fledged bio-based economy, in which all agricultural waste streams are used and do not suffice to cover the demand of feedstocks to produce fuels and materials. Optimized selection of designated crops will also need to take into account climatic conditions. For example, miscanthus is sensitive to low temperatures and is therefore not an option for all countries of EU-15, let alone of EU-25. In many of this cases, poplar (or possibly other, more suitable crop plants) could be chosen.

Assumptions on the economics of fermentable sugars

So far, we have only discussed environmental aspects related to the production of fermentable sugar. The economics of these feedstocks are not analyzed in detail in the BREW study. Instead, we simply assume various price levels for fementable sugar. These price levels have been chosen in view of the current production and market prices.

Today, the prices of fermentable sugar differ decisively between the various geographical regions. Particularly low prices are found in Brazil, where the price of sugar from cane was

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the higher land use requirements are a direct consequence of the relatively low overall yields (7 t/ha/a). For maize stover, the low values are a consequence of the economic allocation where maize kernels have a much higher value than maize stover. This illustrates that the use of agricultural waste streams (like stover) requires relatively little land (Table 3-5). We conclude that, among the lignocellulosic feedstocks, priority should be given to the use of waste streams from the perspective of land use. If dedicated crops are used for lignocellulosic feedstocks, then only the crops with very high yields are similarly efficient in terms of land use as dextrose or sucrose.

[44] This is a robust statement because the results for the three allocation approaches for C_5/C_6 sugars have rank No. 2, 3 and 4 for NREU and No. 2, 3 and 5 for NR GHG.

around 70 US$/t in 2000 (see Table A5-1 in Appendix A6). The main reasons for this low price level are the favorable climatic conditions, land availability/ownership and the very low wages in developing countries (wages are especially low in Brazil while higher wages in other developing countries with tropical climate result in larger production costs, see Table A5-1 in Appendix A6). In the next decades, wages in low-income countries are expected to increase parallel to economic development and industrialization. In Brazil, a significant rise in demand for sugar cane for domestic bioethanol production is lately leading to increased world market prices for sugar. In September 2005 this world market price for sugar was around 330 US$/t (see Figure A6-1 in Appendix A6).

In the USA and in Europe, the fermentable sugar price is around 200 – 300 €/t. The price of 300 €/t represents the current price of sugar made from starch crops in Europe where the cereals price is around the world market price. Sugar production from beet in Europe is decisively more expensive, costing around 700 €/t but the higher production cost is currently compensated by subsidies (around 400 €/t). These subsidies for sugar beet will be gradually removed over the next few years. As a consequence, sugar industry in Europe will be restructured shifting from sugar beet to starch as raw material.

In view of this range of prices, the price levels for fermentable sugar assumed in BREW tool are 70, 135, 200 and 400 €/t.

3.4.2 Techno-economic analysis of 1,3-PDO as exemplary case for fermentation

In this section the results of the environmental and the economic assessment are presented for 1,3-propanediol (PDO). Analogous analyses were performed for all studied products that are manufactured by fermentation (see Table 3-2 for an overview). The results for all fermentation products are discussed in condensed form in Section 3.4.3 (environmental analysis) and Section 3.4.4 (economic analysis). One reason for presenting PDO in this Section is that both production routes are currently being pursued by industry: Shell produces PDO from petrochemical ethylene via ethylene oxide, whereas DuPont is currently building a plant for PDO production from maize-based glucose; this indicates that both the bio-based and the petrochemical production are economically viable and it raises the question which route is preferable from an economic point of view. Another reason for presenting PDO in more detail in this chapter is that various data sources were available: Apart from results generated with the Generic Approach, original company data were provided by DuPont (for both their bio-based process and for the petrochemical Degussa process), a study prepared by SRI was available (SRI-PEP227) and some process data were found in the open literature (esp. Grothe 2000).

Environmental assessment of PDO

Figure 3-8 shows the cradle-to-factory gate energy requirements for the production of 1,3-propanediol (PDO) from maize starch, glycerol and petrochemicals. The first five bars from the left (TODAY) represent maize starch-based processes using current technology. The underlying data originate from the companies (SRI data were made available on a confidential

basis for the purpose of this project) or from the Generic Approach (GA, denoted with a capital "T" for TODAY). The following two bars display the results for maize starch-based processes using future technology (denoted with a capital "F"). The underlying data originate exclusively from the Generic Approach (GA); both progress in fermentation (see Table 3-2) and in product separation and purification have been assumed. The fourth and fifth bar from the right represent fermentation processes based on glycerol and using state of the art technology. Finally, the three bars on the far right show the results for petrochemical processes using current technology but different petrochemical feedstocks, namely ethylene (via ethylene oxide), acrolein (from propylene) and propylene (most likely via acrolein).

The key features of the process flow diagrams for all cases shown in Figure 3-8 are summarized in Box 3-2 and the attendant process flow diagrams are given in Appendix A9. It should be noted that there are differences in the quality of the data used for the calculations, with process data originating from large-scale plants being most reliable. Our Generic Approach and desktop studies such as the reports by SRI rely on a variety of sources and our assumptions and the resulting estimates are meant as best possible approximations. While, by use of BREWtool, a uniform methodology is applied and a common dataset is being used, smaller inconsistencies are unavoidable (e.g., because some of the data provided by the companies and institutes were aggregated). For these reasons, (smaller) differences in the results presented below should not be overinterpreted.

The comparison of the results based on company data (bar 1-3) with those based on the Generic Approach for current technology (bar 4-5) show a fair correspondence, indicating the validity of the Generic Approach. The results based on application of the Generic Approach for the future (bar 6-7) show that depending on the technological progress the savings of non-renewable energy can be very substantial. Bar 7 (BioPDO-Aer-GA-FpvH2O) represents a process scheme that combines a highly efficient biotechnological step (see Table 3-2) with product separation using a membrane that is selective for PDO. The production by fermentation of glycerol according to the current state of the art (bar 4-5 from the right)[45] requires more non-renewable energy than state of the art processes based on maize starch (bar 1-5). More advanced processes using diluted instead of pure glycerol may improve the performance of this route but could not be assessed due to lack of data. The glycerol-based processes and – even more so – the maize-based processes require clearly less non-renewable energy than the current petrochemical processes (bar 1-3 from right). Of all processes studied, the non-renewable energy requirements are lowest for the state-of-the art process BioPDO-Aer-GA-Tevcont and for the future process BioPDO-Aer-GA-FpvPDO.[46]

[45] The solid bars for the glycerol cases refer to price allocation. The upper value (of the error bars) for the glycerol cases refer to mass allocation.
SRI provides process data for the conversion of glucose to PDO via glycerol. As first approximation, we assume this data to be representative also for the conversion of glycerol to PDO. Due to the dominance of downstream processing for the overall energy use the error made is expected to be low.

[46] At first sight, it is unexpected that the NREU of the future process BioPDO-Aer-GA-FpvH2O is larger than that of BioPDO-Aer-GA-Tevcont, which is based on today's technology. The (gross) energy requirements are approximately identical but the reason for the difference is that less biomass is produced in the future process (BioPDO-Aer-GA-FpvH2O) due to the more efficient fermentation and as a consequence, the energy credit from the waste biomass is smaller. On the other hand, the advantage is that less land is needed for BioPDO-Aer-GA-FpvH2O (see Figure 3-12).

1. BioPDO-Anaer-SRI-Tdcont: Current technology (TODAY); anaerobic continuous process based on glucose; workup by evaporation/crystallization and distillation; data from SRI (SRI-PEP 227, 1999).
2. BioPDO-Aer-SRI-Tdcont: Current technology (TODAY); aerobic continuous process based on glucose; workup by evaporation/crystallization and distillation; data from SRI (SRI-PEP 227, 1999).
3. BioPDO-Aer-DP-Tu: Current technology (TODAY); aerobic process; further details on the fermentation and the product workup are confidential; confidential data from DuPont.
4. BioPDO-Aer-GA-Tevbat: Current technology (TODAY); aerobic batch process based on glucose; workup by evaporation of water followed by evaporation and distillation of PDO; Generic Approach.
5. BioPDO-Aer-GA-Tevcont: Current technology (TODAY); aerobic continuous process based on glucose, otherwise identical with No.4; Generic Approach.
6. BioPDO-Aer-GA-FpvH2O: FUTURE technology; aerobic continuous process based on glucose; separation by pervaporation of water and distillation of PDO; Generic Approach.
7. BioPDO-Aer-GA-FpvPDO: FUTURE technology; aerobic continuous process based on glucose; separation by pervaporation and distillation of PDO; Generic Approach.
8. BioPDO-Anaer-Glyc-SRI-Tdcont: Current technology (TODAY); anaerobic continuous process; glycerol as feedstock while No. 1-6 are based on glucose; separation by evaporation/crystallization and distillation; data from SRI (SRI-PEP 227, 1999).
9. BioPDO-Anaer-Glyc-VDI-Tdbat: Current technology (TODAY); anaerobic batch process; glycerol as feedstock while No.1-6 are based on glucose; separation by distillation; data from Grothe (2000)/VDI.
10. PchemPDO-EO-SRI: Current technology (TODAY); petrochemical process based on ethylene oxide (hydroformulation of ethylene oxide; ethylene oxide from ethylene); data from SRI (SRI-PEP 227, 1999).
11. PchemPDO-Acro-SRI: Current technology (TODAY); petrochemical process based on acrolein (hydration of acrolein; acrolein via oxidation of propylene; this is the process operated by Shell Chemicals); data from SRI (SRI-PEP 227, 1999).
12. PchemPDO-Propyl-DP: Current technology (TODAY); petrochemical process based on propylene; further details on the process are confidential; confidential data from DuPont (bought patent from Degussa).

Box 3-2: Key features of the process flow diagrams for all processes studied for 1,3-propanediol (PDO; for all other products see Appendix A8)

For practically all bio-based processes, the *total* of renewable energy *and* non-renewable energy is larger than the requirements of non-renewable energy in the petrochemical process via ethylene oxide (PchemPDO-EO-SRI).[49] This can be explained with the generally high selectivity of petrochemical processes and the absence of water, the removal of which is an important driver for energy use in bio-based fermentation processes. However, the petrochemical processes via acrolein (PchemPDO-Acro-SRI) and via propylene (PchemPDO-Propyl-DP) are not or hardly more favourable with regard to *total* energy use (total of renewable and non-renewable energy) compared to the bio-based processes. Moreover, the error bar shown above the bar for ethylene oxide-based PDO (PchemPDO-EO-SRI) indicates the uncertainty of this conclusion even for this process.

The error bar for ethylene oxide-based PDO also indicates that the advantage of the bio-based processes may be very substantial. The upper value indicated by the error bar for ethylene-oxide based PDO (approx. 125 GJ/t) has been derived from data published by Shell's on polytrimethylene terephthalate (PTT; Elliot et al. 2005). The estimate of 125 GJ/t does not necessarily coincide with Shell's own calculations for 1 t PDO (the real values determined by Shell have not been disclosed); we calculated it by using the results published by Shell for polytrimethylene terephthalate (PTT) and subsequently deducting the polymerisation step and the production of purified terephthalic acid as assumed in the BREW calculations.[50]

The indicator *non-renewable energy use* (NREU) for the system cradle-to-factory gate (Figure 3-8) is identical with the indicator NREU for the system cradle-to-grave under the condition that waste PDO is incinerated without energy recovery (not depicted).[51] In the case of waste incineration *with* energy recovery and in the case of digestion with energy recovery, constant values (representing the extent of energy recovery) are deducted for all products. The relative position of the various processes according to the indicator *non-renewable energy use* (NREU) is hence identical with and without energy recovery. The indicator *non-renewable energy use* (NREU) shown in Figure 3-8 has therefore a key role for the interpretation of the environmental impacts of a product.

Figure 3-9 illustrates the calculation procedure for (net) *GHG emissions for the system "cradle-to-factory gate" (GHG emissions)*: The starting point for calculating these net GHG emisissions are the (gross) *GHG emissions originating from non-renewable energy use (NRGHG)*.[52] If we subtract from these emissions (NRGHG) the CO_2 equivalents of the

[49] The process BioPDO-Aer-GA-FpvPDO is an exception; here, the large energy credits originating from the combustion of energy byproducts lead to a total energy use (total of renewable and non-renewable energy) that is smaller than the non-renewable energy input in petrochemical processes.

[50] Therefore, the derived value of 125 GJ/t may differ from the results determined by Shell for PDO for two reasons:

a) Different assumptions between the calculations by Shell and those performed in the BREW study with regard to energy use and emissions for both the production of purified terephthalic acid and for the polymerisation step.
b) Different process data used for PDO production (own Shell data versus SRI data as used in BREW).

[51] As a further condition, the energy required for waste transportation from the consumer to the waste management facility must be negligible which is typically the case.

[52] These emissions (NR-GHG) follow the same pattern as the non-renewable energy use (NREU) according to Figure 3-8. Differences in the pattern can be caused by different fuel mixes depending on the source (share of natural gas and oil products in fuel); moreover, GHG emissions include also process-related greenhouse gases which are not related to energy use (especially the CO_2 equivalents of the N_2O emissions originating from fertilizer use)

renewable carbon embodied in the product (bars with negative values) the result are the (net) *GHG emissions* for the system "cradle-to-factory gate". Interestingly, the value for the case BioPDO-Aer-GA-FpvPDO becomes negative (Figure 3-9). The reason is that the gross GHG emissions from non-renewable energy use are smaller than the CO_2 equivalents sequestered in PDO.

Instead of studying the system "cradle-to-factory gate" it should be our preference cover the entire life cycle. In terms of LCA computation the easiest way to do so is to assume *incineration without energy recovery* (PDO is not incinerated as such but only in a chemically converted form, e.g. in the plastic PTT). For (fully) bio-based products, the values for *incineration without energy recovery* in Figure 3-10 are identical with the (gross) *cradle-to-factory-gate GHG emissions originating from non-renewable energy use (NRGHG)* according to Figure 3-9. For petrochemical products, the fossil carbon embodied in the products needs to be added to these emissions (NRGHG) in order to arrive at the values for *incineration without energy recovery* according to Figure 3-9.

As mentioned in Section 3.2.5, end-of-life considerations as depicted in Figure 3-10 are irrelevant for chemical intermediates (such as PDO) from a practical point of view because only end products that reach the consumer and are discarded by him/her can be treated in waste management plants. Nevertheless waste management calculations are performed for all products studied in the BREW project in order to understand the importance of this stage in the process chain. Moreover, we conduct for all products end-of-life calculations for incineration with and without energy recovery and for digestion (see Figure 3-10), even though digestion is only relevant for biodegradable compounds.

For all cases depicted in Figure 3-10, the values for *incineration with energy recovery* differ by a constant value from those for *incineration without energy recovery* (compare Section 3.2.5). Likewise, the values for *digestion with energy recovery* differ by a constant value from those for *incineration without energy recovery*. The overall pattern of Figure 3-10 coincides with that of *non-renewable energy use* (NREU) for the system cradle to factory gate according to Figure 3-8. This underlines that the *non-renewable energy use* (NREU) for the system cradle-to-factory gate can be seen as key indicator as it was already pointed out earlier in this section. We therefore choose this indicator and express the savings of NREU of all fermentation processes relative to one of the petrochemical processes that is chosen as benchmark (here: the ethylene route, PchemPDO-EO-SRI): As shown in Figure 3-11 the saving potentials offered by bio-based PDO are 30% ± 10% TODAY and 55% ± 20% in the FUTURE.

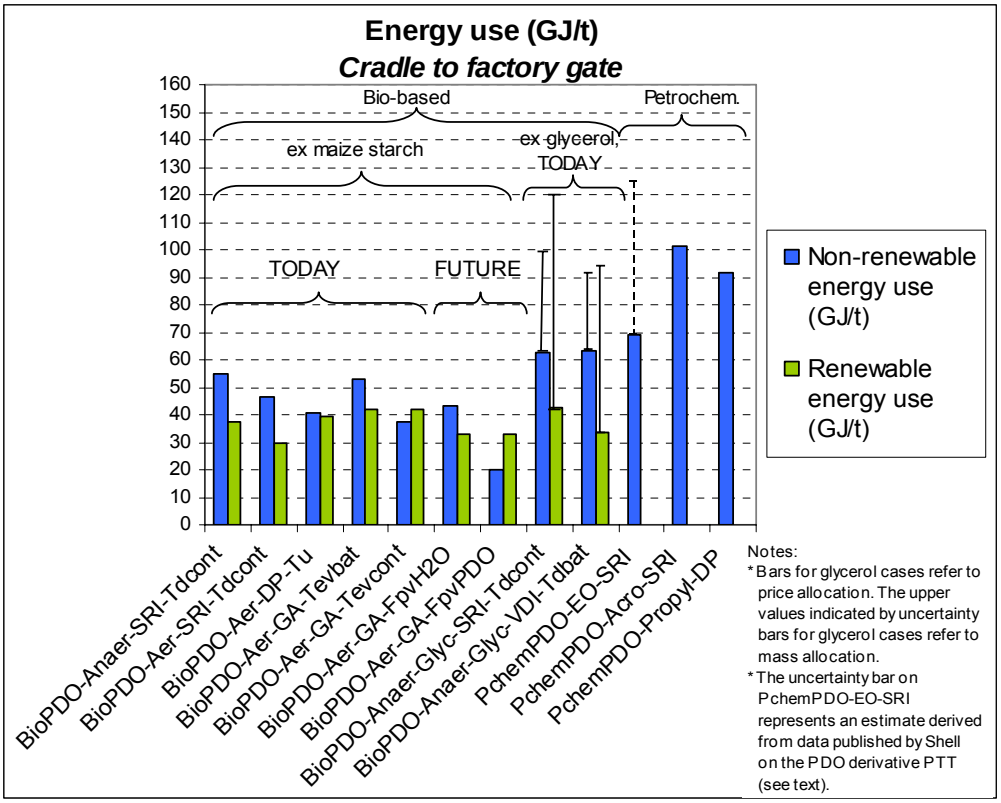


Figure 3-8: Cradle-to-factory gate energy use of 1,3-propanediol from maize starch, glycerol and petrochemicals

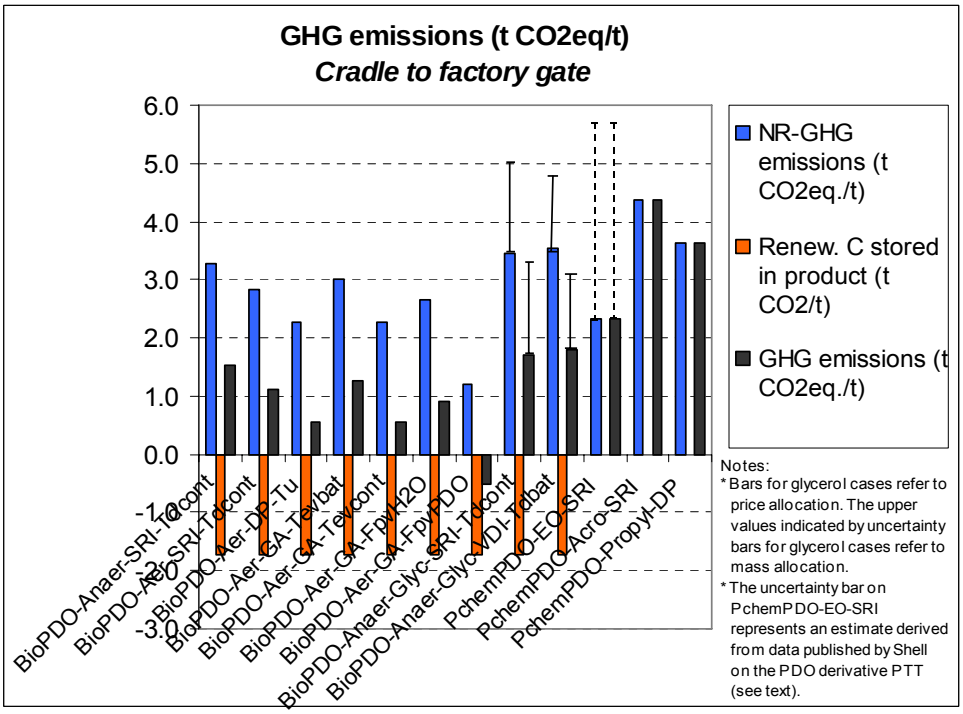


Figure 3-9: Cradle-to-factory gate GHG emissions of 1,3-propanediol from maize starch, glycerol and petrochemicals

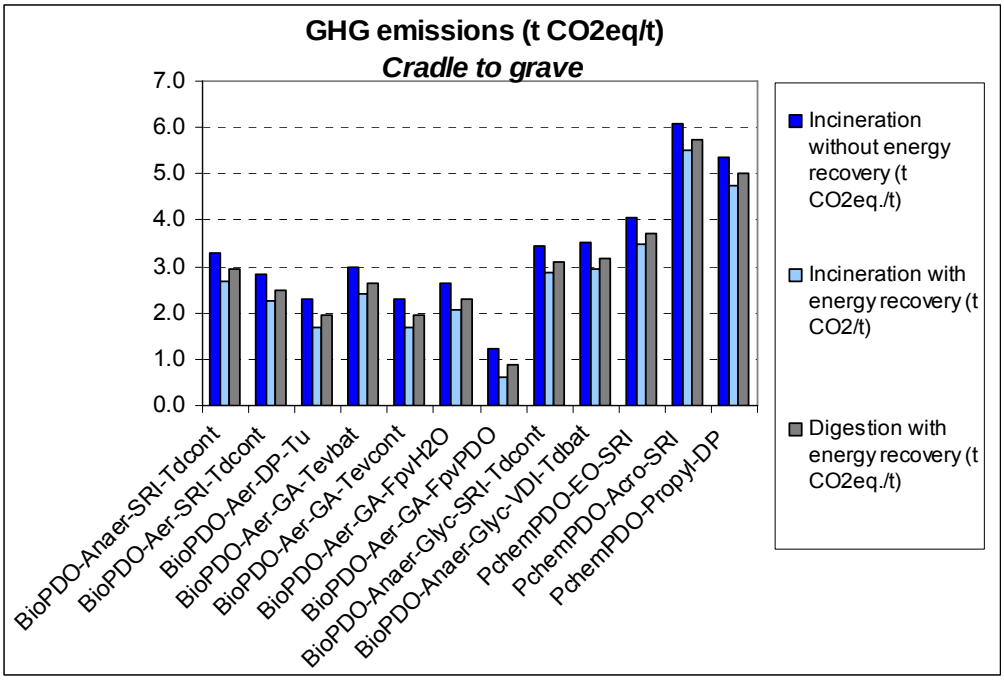


Figure 3-10: Cradle-to-grave GHG emissions of 1,3-propanediol from maize starch, glycerol and petrochemicals (error ranges are not displayed; the same error ranges as those shown in Figure 3-9 apply)

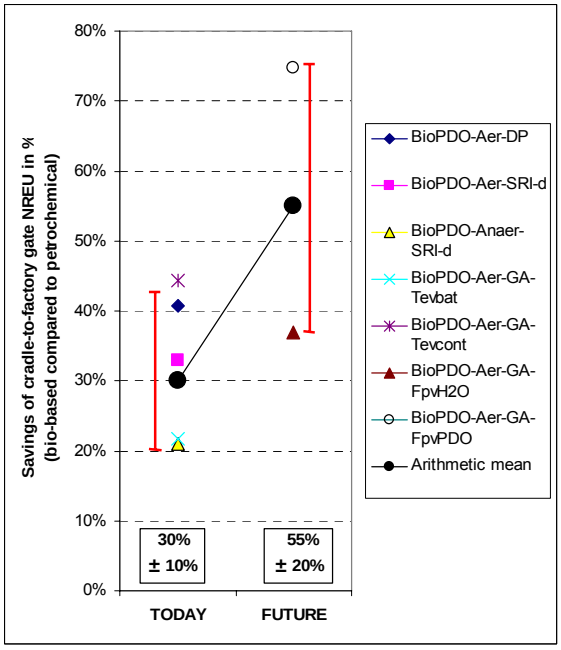


Figure 3-11: Saving potentials of cradle-to-factory gate NREU for the production of 1,3-propanediol from maize starch relative to petrochemical PDO (PDO from glycerol is not depicted in this figure; petrochemical PDO chosen as benchmark: PchemPDO-EO-SRI, NREU = 69.1 GJ/t; see Figure 3-8)

While the indicators *non-renewable energy use* (NREU) and *emissions originating from non-renewable energy use (NRGHG)* are interlinked, land use is an independent parameter. Land use is, however, closely linked to renewable energy use. Since products and processes using renewable raw materials are more frequently assessed on the basis of land use and derived indicators, we pay in this report more attention to land use than to renewable energy use. The results for land use shown in Figure 3-12 refer exclusively to agricultural land, which explains why the values are zero for petrochemical PDO. It is justified to neglect the land requirements for chemical plants and transporation infrastructure because firstly, these values are comparable for bio-based and for petrochemical products (they therefore cancel out) and secondly, they are relatively small compared to agricultural land.

The differences in land use for the first six cases in Figure 3-12 (all these cases are based on starch crops) are a direct consequence of differences in product yields in the fermentation step. The relatively small differences in land use for all process routes based on maize starch (bar 1-7) hence reflects the limited scope to improve the fermentation yields beyond the current-state-of the art even under the condition of substantial R&D over 2-3 decades (compare Table 3-2). This phenomenon is found also for most other products studied (see below) leading to the conclusion that no major improvements are to be expected in terms of land use efficiency if starch crops are used.

Contrary to the first seven bars in Figure 3-12, clearly larger amounts of land are needed if glycerol is chosen as fermentation substrate.[53] This is only to a small extent caused by lower fermentation yields; the main reason is that land use per tonne of substrate is larger for glycerol. Excluding the glycerol-based cases, the land requirements are between 0.2 and 0.3 ha per tonne of PDO (bar 1 to 6 in Figure 3-12). This is quite representative for most chemicals made from starch as will be shown below (Figure 3-17).

Compared to the use of glycerol and of starch-based fermentable sugar, the use of non-renewable energy (NREU) can be clearly reduced if fermentable sugar is made from lignocellulosics or from sugar cane. This has been discussed in general terms in Section 3.4.1 and it is demonstrated in Figure 3-13 for a future case of PDO production (pervaporation of water, BioPDO-Aer-GA-FpH2O). As shown there, the potential savings of non-renewable energy use (NREU) by switching from starch-based PDO (case F) to PDO made from lignocellulosics (case C) are 15 GJ/t PDOor 45% (comparison for default cases). Switching from lignocellulosics to sugar cane allows additional savings of another 16 GJ/t PDO, i.e. by another 65% (comparison for default cases).

As discussed in Section 3.4.1, the 20%-economic-allocation can be seen as approximation for supply of fermentable sugar from sugar cane without co-production of power (by incineration of the bagasse). The 20%-economic-allocation is represented by case B in Figure 3-13. The comparison with the other cases shown in Figure 3-13 shows that, by not making use of the calorific value of bagasse for power generation, sugar cane looses its clearly advantageous position (transition from case A to case B) and takes an intermediate position between lignocellulosics (cases C and E) and starch (cases F and G).

While Figure 3-13 refers to a specific process scheme for the future (BioPDO-Aer-GA-FpH2O) the savings in relative terms by replacing starch-based feedstocks by fermentable

[53] The bars for glycerol cases refer to price allocation. Mass-based allocation would increase the land use of glycerol-based PDO by a factor of 3. This factor of three represents the prices used in the allocation method (approx. 600 €/t for biodiesel vs. approx. 200 €/t for crude glycerol).

sugars from lignocellulosics or sugar cane are very comparable for other process schemes for PDO. The savings for non-renewable greenhouse gas emissions (NRGHG) also follow a similar pattern. However, it should be kept in mind that the production of fermentable sugars from lignocellulose and their use as fermentation feedstock is not yet technologically proven, while the production of fermentable sugars from starch crops and sugar cane represents the state-of-the art.

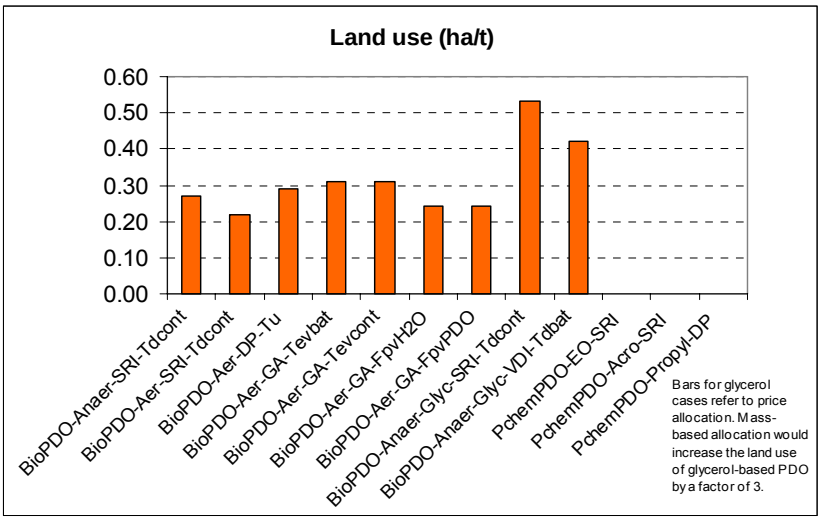
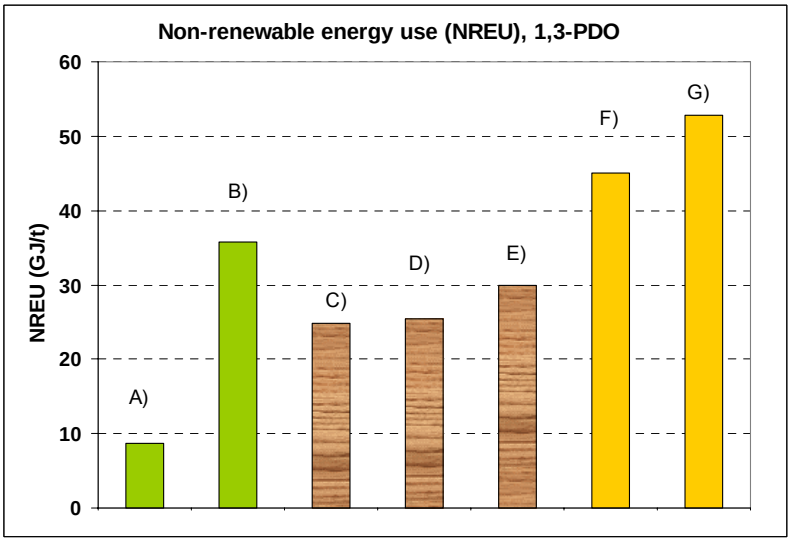


Figure 3-12: Land use requirements for the production of 1,3-propanediol from maize starch, glycerol and petrochemicals



A) Sugar cane, default (energy credit)
B) Sugar cane, sensitivity (econ. allocation, 20%)
C) Lignocellulosics, default (econ. allocation)
D) Lignocellulosics, sensitivity miscanthus
E) Lignocellulosics, sensitivity poplar
F) Maize starch, default
G) Maize starch, sensitivity (high energy use)

Figure 3-13: Cradle-to-factory gate NREU for the production of 1 tonne of 1,3-propanediol (PDO) - Sensitivity analysis for different feedstock types and allocation procedures (example chosen: Generic Approach, FUTURE case with pervaporation of water, BioPDO-Aer-GA-FpH2O)

If a given process saves non-renewable energy and and has low GHG emissions, this may be due to a highly efficient conversion in the biotechnological step and/or due to very efficient downstream processing. However, it is also possible that the biotechnological step is rather inefficient, leading to large amounts of biomass in the fermentation process. If this biomass is burnt to produce heat and electricity the quantities may be large enough to cover a considerable share of the (high) process energy requirements or even to overcompensate this disadvantage. Such cases are characterized by relatively large land requirements. Since the two parametres *can* - but do not necessarily *have to* – be linked, it is important to simultaneously analyze NREU (or GHG emissions) and land use, in addition to the separate analyses discussed above. For simultaneous analysis, the ratio of saved NREU (compared to the conventional case) and the land requirements can be determined. As shown in Figure 3-14 for starch and glycerol-based PDO, rather attractive processes save around 100 GJ NREU per hectare land and the most advanced future scheme (BioPDO-Aer-GA-FpvPDO) offers savings of somewhat more than 200 GJ NREU per hectare land. For comparison, the horizontal broken lines in Figure 3-14 represent the maximum NREU savings by use of short-rotation poplar and miscanthus for co-combustion in coal-based power plants . The value for miscanthus can be seen as the highest possible value achievable with bioenergy because miscanthus has outstandingly high yields under suitable conditions (the value of 230 GJ/ha/a according to Figure 3-14 is based on the assumption of a yield of 14 t_{dm}/ha/a, a higher heating value of 19.2 GJ/t and an estimated energy share of 15% for drying, transportation and preprocessing).However, the climatic conditions are not adequate for miscanthus throughout Europe and the fact that the yields in the first year are low is a disadvantage. The value for poplar (110 GJ/ha/a) can be seen as more generally achievable value (based on a yield of 7 t_{dm}/ha/a, a higher heating value of 18.5 GJ/t and 15% for drying, transportation and preprocessing). The comparison in Figure 3-14 indicates that the non-renewable energy savings for bio-based PDO production per unit of agricultural land are comparable to those for power production from poplar for about half of the PDO process designs (based on maize starch) while the remainder is less attractive. If cultivation of miscanthus is possible with an average yearly yield of 14 t_{dm}/ha, power generation from miscanthus is much more attractive than PDO from maize in terms of non-renewable energy savings per unit of land.

Instead of comparing the two bioenergy options to PDO from maize starch they can also be compared to PDO derived from poplar and from miscanthus; the result of this comparison (not shown in Figure 3-14) is that the NREU savings per unit of land are comparable. [54]

Finally, it is interesting to make a comparison with *fuel* ethanol because liquid biofuels are in the focus of attention of policy makers nearly worldwide (Berg 2004). Maize-based *ethanol for fuel purposes* offers only comparatively small savings in the order of 20-30 GJ/ha/a. This range has been checked against various sources.[55] It is important to realize that these savings,

[54] Since the production of fermentable sugar from lignocellulosics (poplar, miscanthus) is not yet technologically feasible, the comparison is only made for the FUTURE cases of PDO production. Assuming, firstly, poplar as raw material for the fermentable sugar, we calculate NREU savings of 80 GJ/ha/a for BioPDO-Aer-GA-FpvH2O and of 140 GJ/ha/a for BioPDO-Aer-GA-FpvPDO; this range is rather close to the value for the bioenergy use of poplar according to Figure 3-14 (110 GJ/ha/a). Assuming, secondly, miscanthus as raw material for the fermentable sugar, we calculate NREU savings of 180 GJ/ha/a for BioPDO-Aer-GA-FpvH2O and of 290 GJ/ha/a for BioPDO-Aer-GA-FpvPDO; this range is in the vicinity of the value for the bioenergy use of miscanthus according to Figure 3-14 (230 GJ/ha/a).

[55] For comparison:

- The following calculation yields estimated savings of non-renewable energy use of approximately 20 GJ/ha/a for ethanol from maize:
  - According to Shapouri et al. (2002) the net savings related to the use of ethanol from maize as substitute for petrol amount to 25%-30% of the calorific value of ethanol (Table 1, last row in Shapouri

which are related to the use of bioethanol for *fuel purposes*, are smaller than by bioethanol for *chemical* purposes. The reason is that bioethanol for fuel purposes replaces petrol (gasoline) while bioethanol for chemical purposes replaces chemical ethanol with a longer supply chain and larger overall energy requirements (NREU) than petrol:

- In terms of heating values, one tonne of bioethanol for fuel purposes is equivalent to 0.69 t petrol. With an assumed energy-requirements-for energy (EFE) of 7% for the extraction, refining and transportation of crude oil and petrol, the related the cradle-to-consumer energy requirements amount to 0.69 x 1.07 x 45.8 (higher heating value of petrol) = 33.7 GJ. According to our own calculations it requires approximately 27 GJ non-renewable energy (range: 24-30 GJ, see Table 3-7, part 1) to make 1 tonne bioethanol. Therefore, the net savings are around 6.5 GJ NREU/t ethanol (=33.7 – 27.2).[56]
- In contrast, if one tonne of bioethanol replaces petrochemical ethanol, the cradle-to-factory energy requirements for the production of 1 t petrochemical ethanol is saved; these are estimated at 54-64 GJ (see Table 3-7, PchemEtOH-1 and PchemEtOH-2). Assuming again that it requires approximately 27 GJ non-renewable energy to make 1 tonne bioethanol, the savings are between 27 and 37 GJ/t ethanol.

This gives an advantage of a factor of 4 to nearly 6 in favour of bioethanol use for chemical purposes as compared to fuel purposes. We said above that *fuel* ethanol from maize offers savings in the order of 20-30 GJ/ha/a. By multiplication by a factor of four to six we estimate the energy savings for *chemical* ethanol to be in the range of 100 to 150 GJ/ha/a.[57] This range of values is confirmed later in this study (Figure 3-19).

The obvious conclusion to use bioethanol for chemical purposes instead of fuel has practical limits because the amount of ethanol used in petrochemical industry today is relatively small: We estimate that total current ethanol use in Europe is in the range of 1 to 2 million tonnes,

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et al., 2002: 21,105 BTU/gal saved divided by the Higher heating value of ethanol, i.e. 83.961 BTU/gal gives 25%). This means that for each GJ ethanol substituting petrol, 0.25 GJ fossil energy is saved. Accounting for extraction, refining and transport of crude oil/petrol adds rougly another 0.05 GJ, resulting in total savings of 0.30 GJ fossil energy for each GJ ethanol replacing petrol).

- A yield of 3200 l ethanol per hectare is quite representative for ethanol production from maize (Berg 2004). It translates to 2250 litres of gasoline equivalents per haor to 0.44 ha per 1000 l gasoline equivalent (the latter is confirmed by OECD, 2006). Due to co-production of other products from maize, one may argue that not all of the land use should be allocated to the maize starch which are converted to ethanol. Applying the data developed by Vink et al. (forthcoming b) gives 33% larger ethanol yields, i.e. approximately 4250 l ethanol per hectare instead of 3200 l.
- 3200 l ethanol per hectare is equivalent to 75 GJ ethanol produced per hectare. And 4250 l ethanol per hectare is equivalent to 100 GJ ethanol produced per hectare. Multiplication by the net savings mentioned above for the net savings using ethanol as substitute for petrol (25%-30%) gives a value of around 20 GJ fossil energy saved per hectare (range: 18.75 – 22.5) for 3200 l ethanol per hectare and around 27.5 GJ fossil energy saved per hectare (range: 25.0 – 30.0) for 4250 l ethanol per hectare. The overall range is therefore 20-30 GJ fossil energy saved per hectare. For comparison, the next bullet points give the savings per hectare according to other authors, including also other agricultural crops.

- Schmitz (2005; p.258) estimates the savings of non-renewable energy use per hectare at approximately 16 GJ/ha/a for ethanol from maize, at approximately 12 GJ/ha/a for ethanol from wheat and at around 85 GJ/ha/a for ethanol from sugar beet.
- Stelzer (1999; quoted in Schmitz, 2005, p.191) estimates the savings of non-renewable energy use per hectare at 33 GJ/ha/a for ethanol from wheat and at 71 GJ/ha/a for ethanol from sugar beet.
- Kaltschmitt and Reinhardt (1997) estimate the savings of non-renewable energy use per hectare at approximately 30 GJ/ha/a (15-50 GJ/ha/a; p.392) for ethanol from wheat, at 30-80 GJ/ha/a for ethanol from potatoes and an average of 80 GJ/ha/a (50-140 GJ/ha/a; p.381) for ethanol from sugar beet.

[56] Shapouri et al. (2002) provide a whole range of values derived from the literature. According to their own calculations 22.2 GJ are required to produce 1 t ethanol (netted off co-products). This results in net energy savings are around 11.5 GJ NREU/t ethanol (=33.7 – 22.2).

[57] Using the data calculated by Shapouri et al. (2002), an advantage of a factor of 4 is calculated in favour of bioethanol use for chemical purposes as compared to fuel purpose.

while a 5-30% ethanol/petrol blend would require 15-90 million tonnes of ethanol. Nevertheless the conclusion that bioethanol use for *chemical* instead of *fuel* purposes offers larger saving potentials in GJ per hectare is useful because it may also apply also to other many White Biotechnology chemicals. As shown in Figure 3-14 this is the case for PDO: The grey band shows the primary energy savings by *fuel* ethanol from maize (20-30 GJ/ha/a) while good PDO processes save nearly 100 GJ per hectare. We will show in Section 3.4.3 that this is not only true for PDO but also for many more White Biotechnology chemicals covered in this study (Figure 3-19).

The fact that the use of biomass for the production of liquid biofuels is not a very resource-efficient strategy has been pointed out by numerous other authors. Liquid biofuels score particularly bad in comparison with co-combustion of solid biomass. This is also visible from Figure 3-14.

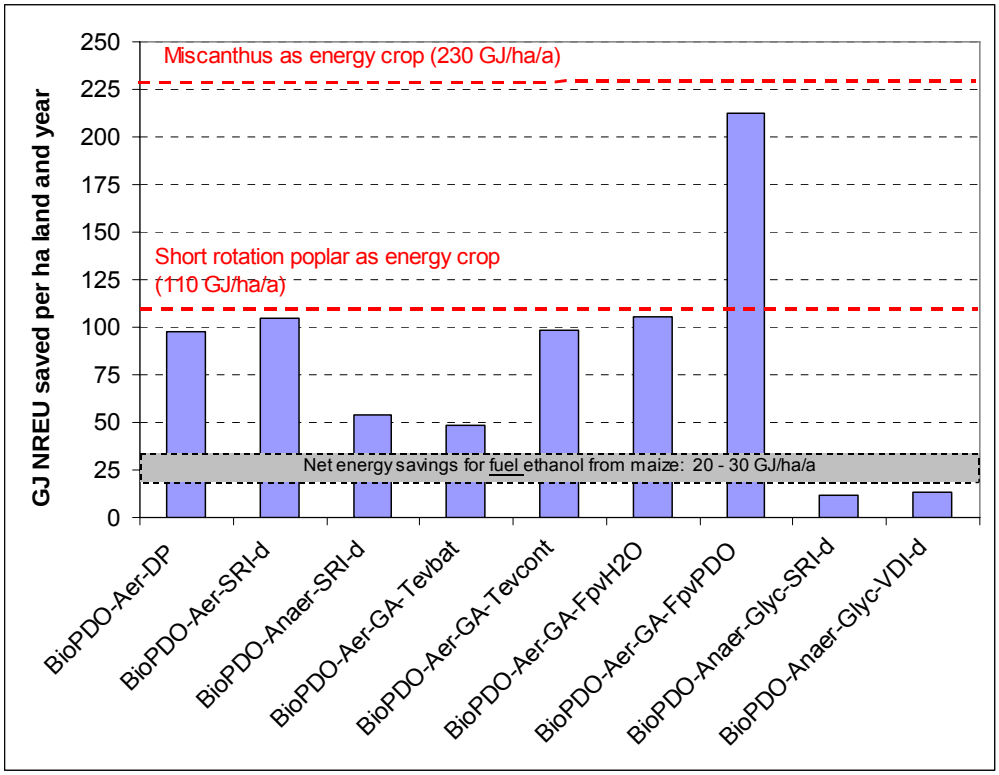

Figure 3-14: Land use efficiency in terms of NREU savings for 1,3-propanediol (PDO) from maize starch - Ratio of savings of non-renewable energy use (NREU savings compared to the petrochemical product) to land used for providing the feedstock for the bio-based product

Economic assessment of PDO

The economic assessment was performed according to the methodology described in Section 3.3.1. Since all fermentation products are based on sugar as a feedstock, the sugar price has a large effect on the production cost and the product value. As explained in Section 3.4.1 (see paragraph titled "Assumptions on the economics of fermentable sugars") four price levels for fermentable sugar were assumed, i.e. 70 €/t, 135 €/t, 200 €/t and 400 €/t, in order to represent a range of prices for both the present and the future. All other prices, such as those for the energy use and for most auxiliaries[58] are kept at present-day values in this Chapter 3 (in contrast, these values and fossil fuel prices will additionally be dynamized in Chapter 4; the key economic assumptions for Chapter 3 are given in Appendix A3-2). The resulting product values are then compared to those of the petrochemical reference products and to market prices in order to determine which of the products and process routes are economically attractive.

Figure 3-15 shows graphically the outcome of the economic analysis, which was conducted in analogy also for all other fermentation products (see below, Section 3.4.5). The curves represent the BREWtool calculation results for bio-based PDO as a function of the price of fermentable sugar, while the horizontal lines give the market price for PDO and the product value of petrochemical PDO (likewise calculated with the method explained in Section 3.3.1). In Figure 3-15 the results are shown for only two processes leading to bio-based PDO (in both cases based on the Generic Approach). The product values for all other process designs studied (compare, for example, Figure 3-8) lie within the range given by these two curves. As an exception, the product values of the processes based on glycerol (BioPDO-Anaer-Glyc-SRI-Td and BioPDO-Anaer-Glyc-VDI-Td) are not included in the bandwidth given by the two curves in Figure 3-15. The glycerol-based processes have been excluded because their production cost is around twice as high as the manufacture by sugar-based fermentation (comparison for TODAY at a sugar price level of 200 €/t and a glycerol price of 700 €/t). Figure 3-8 shows that the product value for petrochemical PDO and the market price differ substantially. The rather high market price (approx. 2400 €/t) reflects the production in relatively small facilities nowadays, the use of the PDO-based polymer polytrimethylene terephthalate (PTT) for higher value applications and the imperfect market conditions (limited number of producers). The product value of petrochemical PDO (for a plant with the capacity of 100 kt p.a. 750-850 €/t according to DSM; 1100 €/t for ethylene oxide-based PDO according to SRI, 1999, scaled to 100 kt) is therefore a more suitable benchmark for bio-based PDO. As shown in Figure 3-15, the process design according to the current state-of-technology (BioPDO-Aer-GA-Tev) is economically feasible compared to petrochemical PDO up to a sugar price between 135 and 200 €/t. The depicted FUTURE process design (BioPDO-Aer-GA-FpvPDO) is economically feasible up to a fermentable sugar price of approximately 400 €/t. In view of the uncertainties of the data used and the method applied we conclude that our economic assessment reflects well that bio-based PDO is very close to commercial viability or is commercially viable already today.

[58] Exceptions are the costs for enzymes and membranes:

- For enzymes, a price level of 100 €/kg was assumed for TODAY and of 10 €/kg for the FUTURE (unless actual prices were available for the specific enzymes used).
- For membrane processes we estimate the membrane cost to be 100 €/tonne bio-based product for TODAY and 50 €/t for the FUTURE.

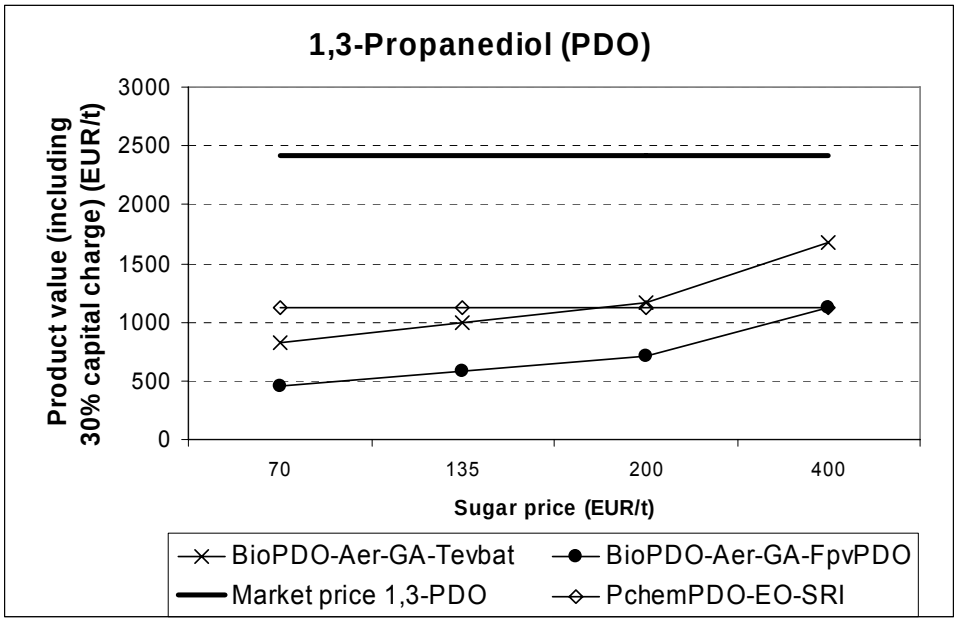

Figure 3-15: Economics of the production of 1,3-propanediol (PDO) depending on the sugar price level and on the level of technology

3.4.3 Overview of the environmental results for all fermentation products

The environmental assessment of all products was carried out according to the methodology explained in Section 3.2.2. The type of results obtained with BREWtool have been described in Section 3.4.2 using PDO as an example. In this section, an overview of the findings across all products is given. We limit ourselves to the discussion of non-renewable energy use (NREU) for the system *cradle-to-factory gate* and to land use (see Table 3-7).[59] Detailed information in tabular form and in diagrams can be found in several appendices: The results for NREU for both the system *cradle-to-factory gate* and *cradle-to-grave*, for greenhouse gas emissions (GHG) and for land use are given in tabular form in Appendix A10. The underlying Process Flow Diagrams and mass balances prepared for the Generic Approach are available in Appendix A9. The flowsheets for the other processes studied are not given in this report for copyright reasons (especially concerning SRI reports) and due to confidentiality (company data). However, Appendix A8 provides short verbal descriptions of all processes (including those analyzed by SRI; comparable to Box 3-2 for PDO, see above), except for those for which also this information is confidential.

According to our calculations it requires in most cases clearly less non-renewable energy (NREU) to produce a given compound from renewable raw materials by means of fermentation than to produce it (or its petrochemical equivalent) via the standard

[59] We do not discuss renewable energy use (REU) because this aspect is indirectly covered via land use (this has been explained in Section 3.4.2). We neither discuss greenhouse gas (GHG) emissions because the pattern of the results for the system *cradle-to-grave* are identical with those for NREU for the system *cradle-to-factory gate* (see also Section 3.4.2). GHG emissions for the system *cradle-to-factory gate* are not discussed because they are considered less relevant from an environmental policy point of view).

petrochemical process (Table 3-7). Figure 3-16 shows the cradle-to-factory gate NREU savings (in %) for maize starch as a feedstock relative to conventional petrochemical production (the calculations conducted for fermentable sugar from sugar cane and from lignocellulosics will be discussed below). Due to limited readability of Figure 3-16 the values are given once more in Table 3-8. Figure 3-16 follows the same concept as Figure 3-11 for PDO (in both graphs the range of values per product is represented by error bars; Figure 3-11 additionally shows the values of the individual processes which constitute the range; the respective data are not given in Figure 3-16 in order to keep the graph readable). In Figure 3-16 ranges for savings are only given for products with more than one workup scheme, provided that the range is at least ±10% (in general, the average value is given and the range is arranged symmetrically around it). For acrylic acid and caprolactam, Figure 3-16 shows results only for the FUTURE because, to our knowledge, the biotechnological production has not been proven so far. No results are given for lactic acid (LA), lysine and citric acid because there is no suitable petrochemical equivalent (petrochemical lactic acid is a speciality because it is a recemic mixture while fermentation-based lactic acid is optically active). For polylactic acid (PLA) and polytrimethylene terephthalate (PTT), the bulk petrochemical product polyethylene terephthalate (PET, amorphous) was chosen as benchmark, while high density polyethylene (HDPE) was chosen in the case of polyhydroxyalkanoates (PHA).[60] In the case of succinic acid, petrochemical maleic anhydride was chosen as reference because this is a commodity while petrochemical succinic acid is a niche product.[61] For bio-based PDO (1,3-propanediol), we chose petrochemical PDO made from ethylene oxide as benchmark.[62] In the case of ethyl *lactate*, which is a green solvent, petrochemical ethyl *acetate* is the petrochemical equivalent.[63] For the ABE process, whose name indicates the products acetone, butanol and ethanol, petrochemical *butanol*[64] was taken as reference because butanol is the main product of the ABE process. All other products shown in Figure 3-16 are commonly produced from petrochemical feedstocks and the respective energy requirements and GHG emissions have been extracted from a variety of sources (primarily from Boustead 1995-2005; Ecoinvent 2003; Patel et al. 1999).

Special caution is required concerning hydrogen (only one data point for TODAY available) for which particularly high NREU savings were found (90%, see Figure 3-16). One important reason is that the microorganisms partly cover their energy requirements with light which was assumed to be primarily daylight; secondly, the feedstock used is a waste stream, i.e. potato slurry proteins, for which no energy intensive pre-processing had to be assumed. It is questionable whether both conditions could be fulfilled at industrial scale. Nevertheless the results indicate promising potentials and call for further research.

[60] All data for these petrochemical polymers were taken from the partial life cycle inventories prepared by Boustead (1999-2005) for the Association of Plastics Manufacturers in Europe.
[61] Having a cradle-to-factory gate NREU value of 96.3 GJ/t, petrochemical succinic acid is clearly more energy intensive to produce than maleic acid which requires 67.7 GJ/t (values estimated based on various sources).
[62] The cradle-to-factory gate NREU of petrochemical PDO has been estimated at 69.1 GJ/t (based on data from SRI 1999).
[63] Based on various sources we estimate the cradle-to-factory gate NREU of ethyl acetate at 59.3 GJ/t. This is clearly lower than the value for benzene (67.7 GJ/t) which could also have been chosen as reference.
[64] Estimated cradle-to-factory gate NREU: 69.3 GJ/t.

		Production system	Non-renewable energy use (NREU), cradle-to-factory gate (GJ/t)			Land use (ha/t)		
			Maize starch	Ligno-cellulosics	Sugar cane	Maize starch	Ligno-cellulosics	Sugar cane
Alcohols	Ethanol	BioEtOH-SRI-Td	27.1	4.4	-13.7	0.28	0.12	0.29
		BioEtOH-SRI-Corn-Td [1)]	24.7	n/a	n/a	0.39	n/a	n/a
		BioEtOH-Anaer-GA-Tdcont	23.9	0.2	-18.7	0.29	0.12	0.29
		BioEtOH-Anaer-GA-Fd	20.4	-2.3	-20.5	0.27	0.11	0.28
		BioEtOH-Anaer-GA-Fpv	18.2	-4.5	-22.7	0.27	0.11	0.28
		BioEtOH-SRI-Stover-Fd [1)]	n/a	22.8	n/a	n/a	0.11	n/a
		PchemEtOH-1 [2)]	63.9	63.9	63.9	n/a	n/a	n/a
		PchemEtOH-2 [2)]	54.2	54.2	54.2	n/a	n/a	n/a
	PDO	BioPDO-Anaer-SRI-Tdcont	54.6	32.3	14.5	0.27	0.11	0.28
		BioPDO-Aer-SRI-Tdcont	46.4	28.4	14.0	0.22	0.09	0.22
		BioPDO-Aer-DP-Tu	40.9	17.1	-2.0	0.29	0.12	0.29
		BioPDO-Aer-GA-Tevbat	53.1	27.4	6.9	0.31	0.13	0.32
		BioPDO-Aer-GA-Tevcont	37.6	11.9	-8.6	0.31	0.13	0.32
		BioPDO-Aer-GA-FpvH2O	43.2	23.1	6.9	0.24	0.10	0.25
		BioPDO-Aer-GA-FpvPDO	19.8	-0.4	-16.5	0.24	0.10	0.25
		BioPDO-Anaer-Glyc-SRI-Tdcont [3)]	62.8	62.8	62.8	0.53	0.53	0.53
		BioPDO-Anaer-Glyc-VDI-Tdbat [3)]	63.5	63.5	63.5	0.42	0.42	0.42
		PchemPDO-Propyl-DP	91.5	91.5	91.5	n/a	n/a	n/a
		PchemPDO-EO-SRI	69.1	69.1	69.1	n/a	n/a	n/a
		PchemPDO-Acro-SRI	101.2	101.2	101.2	n/a	n/a	n/a
	ABE	BioABE-Anaer-GA-Tdcont	63.9	32.5	7.4	0.38	0.15	0.39
		BioABE-Anaer-GA-Tgscont	57.2	25.8	0.7	0.38	0.15	0.39
		BioABE-Anaer-GA-Fdm	29.0	2.6	-18.5	0.32	0.13	0.33
		BioABE-Anaer-GA-Fmd	6.6	-19.8	-40.9	0.32	0.13	0.33
		BioABE-Anaer-GA-Fpv	7.9	-18.5	-39.6	0.32	0.13	0.33
		BioABE-Anaer-GA-Fgs	18.1	-8.3	-29.4	0.32	0.13	0.33
		PchemButanol	69.3	69.3	69.3	n/a	n/a	n/a
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	144.9	123.4	106.3	0.26	0.11	0.26
		BioAcet-Anaer-GA-Ted	108.9	87.7	70.7	0.26	0.11	0.26
		BioAcet-Anaer-GA-FexTOPO	57.4	45.7	36.3	0.14	0.06	0.15
		BioAcet-Anaer-GA-FexDIPE	64.9	52.9	43.3	0.14	0.06	0.15
		BioAcet-Anaer-GA-FedexDIPE	38.9	27.0	17.6	0.14	0.06	0.15
		BioAcet-Anaer-GA-Fed	43.7	31.9	22.5	0.14	0.06	0.15
		PchemAceticAcid	55.5	55.5	55.5	n/a	n/a	n/a
	Acrylic acid	BioAcryl-Anaer-GA-Fex	30.8	16.1	4.4	0.18	0.07	0.18
		PchemAcrylicAcid	47.1	47.1	47.1	n/a	n/a	n/a
	Lactic acid	BioLA-SRI-TpH6cont	37.5	25.4	15.7	0.15	0.07	0.15
		BioLA-SRI-FlowpH	36.8	24.7	15.0	0.22	0.13	0.22
		BioLA-NW-Tu	31.2	18.8	9.0	0.14	0.05	0.14
		BioLA-Sh-Fex	28.5	16.4	6.7	0.22	0.13	0.22
		BioLA-Sh-Fed	30.9	18.8	9.1	0.22	0.13	0.22
		BioLA-Anaer-GA-Fed	22.6	11.0	1.8	0.14	0.06	0.14
		BioLA-NW-Fu	19.6	7.9	-1.5	0.14	0.06	0.14
	Succinic acid	BioSA-Anaer-GA-Tc	66.5	54.5	44.9	0.26	0.17	0.26
		BioSA-Anaer-GA-Ted	27.0	15.0	5.4	0.25	0.17	0.26
		BioSA-Aer-SRI-Fed	45.6	35.1	26.8	0.15	0.08	0.16
		BioSA-Anaer-GA-Fcrx	32.4	22.0	13.6	0.15	0.08	0.16
		BioSA-Anaer-GA-Fc	46.8	37.8	30.7	0.13	0.07	0.14
		BioSA-Anaer-GA-Fed	28.0	17.5	9.1	0.15	0.08	0.15
		PchemMaleicAnhydride	67.7	67.7	67.7	n/a	n/a	n/a
		PchemSA-MalAnhydr	96.3	96.3	96.3	n/a	n/a	n/a
	Adipic acid	BioAdip-Aer-GA-Tc	195.4	134.4	85.7	0.74	0.30	0.75
		BioAdip-Aer-GA-Fc	59.6	37.2	19.4	0.27	0.11	0.28
		BioAdip-Aer-GA-Fed	44.3	21.5	3.2	0.28	0.11	0.28
		PchemAdipicAcid	85.5	85.5	85.5	n/a	n/a	n/a
	Citric acid	BioCit-Aer-SRI-Tevc [4)]	n/a	n/a	73.7	n/a	n/a	0.01
		BioCit-Aer-SRI-Tix	74.9	47.8	26.2	0.33	0.14	0.34
		BioCit-Aer-GA-Tpc	97.0	59.4	29.3	0.45	0.19	0.46
		BioCit-Aer-GA-Fc	22.1	10.7	1.7	0.14	0.06	0.14

[1)] The original process data used covers all steps starting with the intake of corn (for BioEtOH-SRI-Corn-Td) and corn stover (for BioEtOH-SRI-Stover-Fd). For this reason results can only be presented for these two feedstock types.

[2)] Dataset PchemEtOH-1 is b

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics and sugar cane). For this reason the values in this row are identical.

[4)] The original process data used refer to the use of cane molasses. For this reason results are only presented for sugar cane as feedstock type and *not* for maize starch and lignocellulosics. Per tonne of citric acid, 2.6-2.8 tonnes of cane molasses are required. It depends on the allocation approach how much land this translates to (no allocation has been performed here).

Table 3-7, part 1: Cradle-to-factory gate non-renewable energy use (NREU) for fermentation products derived from maize starch, lignocellulosics and sugar cane

			Non-renewable energy use (NREU), cradle-to-factory gate (GJ/t)			Land use (ha/t)		
		Production system	Maize starch	Ligno-cellulosics	Sugar cane	Maize starch	Ligno-cellulosics	Sugar cane
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	43.3	16.0	-5.7	0.33	0.13	0.34
		PchemCapro	117.1	117.1	117.1	n/a	n/a	n/a
	Lysine	BioLys-Aer-SRI-Tix	189.1	160.0	136.8	0.36	0.15	0.37
		BioLys-Aer-SRI-Tsp	65.9	31.9	4.8	0.41	0.17	0.42
		BioLys-Aer-GA-Tix	168.7	120.9	82.8	0.58	0.24	0.59
		BioLys-Aer-GA-Fad	131.1	97.5	70.7	0.41	0.17	0.41
H_2	Hydrogen	BioH2-A&F-gs [1]	14.4	n/a	n/a	n/a	n/a	n/a
		PchemH2	180.0	180.0	180.0	n/a	n/a	n/a
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	64.7	38.3	17.2	0.69	0.51	0.70
		BioPHAmcl-A&F-FA-Oilex [2]	60.9	60.9	60.9	1.88	1.88	1.88
		BioPHA-GA-Toa	37.5	3.4	-23.9	0.41	0.17	0.42
		BioPHA-GA-Th	94.9	61.6	34.9	0.40	0.16	0.41
		BioPHA-GA-Tey	111.6	78.2	51.6	0.40	0.16	0.41
		BioPHA-GA-Tex	91.3	59.1	33.4	0.39	0.16	0.40
		BioPHA-GA-Texey	108.1	75.9	50.2	0.39	0.16	0.40
		BioPHA-GA-OilTexey [2]	109.0	109.0	109.0	1.14	1.14	1.14
		BioPHBV-SRI-Tey-1	143.2	111.5	86.2	0.38	0.16	0.39
		BioPHB-SRI-Tey-2	42.8	11.1	-14.2	0.38	0.16	0.39
		BioPHA-GA-Fey-1	82.3	56.7	36.3	0.31	0.13	0.32
		BioPHA-GA-Fey-2	33.3	7.7	-12.8	0.31	0.13	0.32
		PchemHDPE	76.6	76.6	76.6	n/a	n/a	n/a
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	40.4	1.3	-29.9	0.47	0.19	0.48
		BioEthylene-BioEtOH-Anae-GA-Fpv	31.0	-6.5	-36.5	0.45	0.18	0.46
		PchemEthylene	65.6	65.6	65.6	n/a	n/a	n/a
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	59.5	50.5	43.3	0.16	0.10	0.16
		EL-Sh-pchemEtOH-bioLA-F2	55.6	46.6	39.4	0.16	0.10	0.16
		BioEL-NW-bioEtOH-bioLA-T1	41.3	22.4	7.3	0.22	0.08	0.22
		BioEL-Sh-bioEtOH-bioLA-F3	43.3	34.3	27.1	0.32	0.26	0.32
		BioEL-Sh-bioEtOH-bioLA-F4	43.2	24.5	9.6	0.28	0.14	0.28
		PchemEthylAcetate	59.3	59.3	59.3	n/a	n/a	n/a
		PchemBenzene	67.7	67.7	67.7	n/a	n/a	n/a
		PchemEGBE	73.3	73.3	73.3	n/a	n/a	n/a
		PchemMEK	92.1	92.1	92.1	n/a	n/a	n/a
		PchemAcetone	63.0	63.0	63.0	n/a	n/a	n/a
	PLA	BioPLA-bioLA-SRI-TpH6cont	60.8	45.3	32.9	0.19	0.08	0.20
		BioPLA-bioLA-SRI-FlowpH	59.9	44.4	32.0	0.28	0.17	0.28
		BioPLA-bioLA-NW-Tu	52.7	36.9	24.3	0.18	0.06	0.18
		BioPLA-bioLA-Sh-Fex	49.3	33.8	21.4	0.28	0.17	0.28
		BioPLA-bioLA-Sh-Fed	52.3	36.9	24.5	0.28	0.17	0.28
		BioPLA-bioLA-Anaer-GA-Fed	41.1	26.3	14.5	0.18	0.07	0.18
		BioPLA-bioLA-NW-Fu	40.1	25.1	13.2	0.18	0.07	0.18
		PchemPET Amorph	77.2	77.2	77.2	n/a	n/a	n/a
		PchemPS	86.7	86.7	86.7	n/a	n/a	n/a
		PchemPE LD	77.8	77.8	77.8	n/a	n/a	n/a
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	65.1	58.4	53.1	0.08	0.03	0.08
		PTT-bioPDO-Anaer-SRI-Tdcont	68.1	59.9	53.3	0.10	0.04	0.10
		PTT-bioPDO-Aer-DP-Tu	63.0	54.2	47.2	0.11	0.04	0.11
		PTT-bioPDO-Aer-GA-Tevbat	67.5	58.0	50.5	0.12	0.05	0.12
		PTT-bioPDO-Aer-GA-Tevcont	61.8	52.3	44.7	0.12	0.05	0.12
		PTT-bioPDO-Aer-GA-FpvH2O	63.9	56.4	50.5	0.09	0.04	0.09
		PTT-bioPDO-Aer-GA-FpvPDO	55.2	47.8	41.8	0.09	0.04	0.09
		PTT-bioPDO-Anaer-Glyc-SRI-Td [3]	71.1	71.1	71.1	0.20	0.20	0.20
		PTT-bioPDO-Anaer-Glyc-VDI-Td [3]	71.4	71.4	71.4	0.16	0.16	0.16
		PTT-PchemPDO-Propyl-DP	81.7	81.7	81.7	n/a	n/a	n/a
		PTT-PchemPDO-EO-SRI	73.5	73.5	73.5	n/a	n/a	n/a
		PTT-PchemPDO-EO-Shell	94.6	94.6	94.6	n/a	n/a	n/a
		PTT-PchemPDO-Acro-SRI	85.3	85.3	85.3	n/a	n/a	n/a
		PchemPET Amorph	77.2	77.2	77.2	n/a	n/a	n/a
		PchemNylon-6	120.5	120.5	120.5	n/a	n/a	n/a
		PchemNylon-6,6	138.6	138.6	138.6	n/a	n/a	n/a

[1] The original process data used refer to the use of potato slurry proteins and potato steam peals. These results are reported in the column for maize starch. Per tonne of hydrogen, around 2 tonnes of potato slurry proteins are required. It depends on the allocation approach how much land this translates to (we did not conduct calculations for land use).

[2] This process uses fatty acids (FA) as feedstock for PDO, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil. In our calculations we exclusively assumed rapeseed oil with the typical production characteristics in Europe and assuming a price of rapeseed crude oil of 500 EURO/t. For this reason the values in this row are identical.

[3] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics and sugar cane). For this reason the values in this row are identical.

Table 3-7, part 2: Cradle-to-factory gate non-renewable energy use (NREU) for fermentation products derived from maize starch, lignocellulosics and sugar cane

For all products except for adipic acid, acetic acid and the butanol (ABE process), already TODAY's technology (see left side of Figure 3-16) offers considerable cradle-to-factory gate NREU savings in the range of 20% to over 50%. In the case of butanol, the savings are very small for TODAY and for adipic acid and acetic acid they are even negative, due to the low yield and productivity of the fermentation step. The results for the FUTURE show a particularly large increase in NREU savings especially for these products but also significant improvements for most other products. These improvements, which are based on technological improvement, allow to reach in the FUTURE cradle-to-factory gate NREU savings in the range of 20% up to around 70%.

As Table 3-8 shows the range of achievable savings is particularly large for PHA and for succinic acid for TODAY and for acetic acid, ABE and PDO for the FUTURE (Figure 3-16). However, even considering these uncertainties, the general finding of the existence of considerable NREU saving opportunities both for TODAY and the FUTURE remains robust.

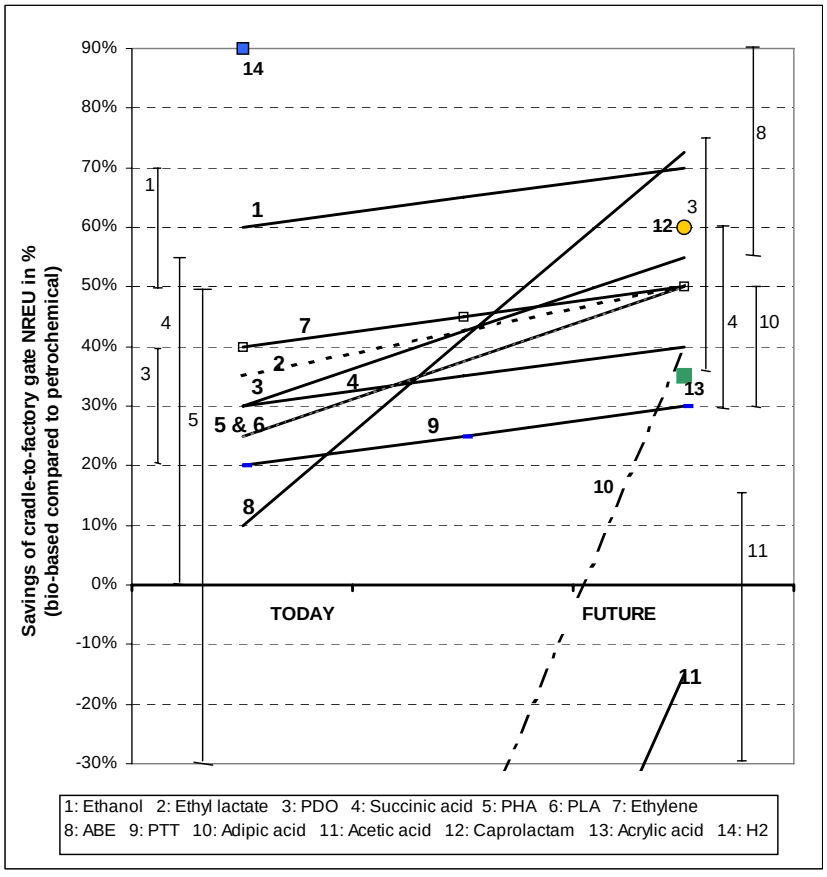

Figure 3-16: Overview of saving potentials of cradle-to-factory gate NREU for fermentation products from maize starch and their derivatives, relative to their petrochemical equivalents (positive values indicate NREU savings for the bio-based process relative to the petrochemical process; for results in tabular form see Table 3-8)

	Savings of cradle-to-factory gate NREU in % (bio-based compared to petrochemical)	
	TODAY	FUTURE
Ethanol	60% (50% to 70%)	70%
PDO	30% (20% to 40%)	55% (35% to 75%)
ABE	10% (5% to 15%)	72.5% (55% to 90%)
Acetic acid	-180% (-140% to - 220%)	-15% (-45% to 15%)
Acrylic acid	n/a	35%
Succinic acid	30% (0% to 55%)	40% (30% to 60%)
Adipic acid	-135%	40% (30% to 50%)
Caprolactam	n/a	60%
Hydrogen	90%	n/a
PHA	25% (-60% to 50%)	50%
Ethylene	40%	50%
Ethyl lactate	35%	50%
PLA	25% (20% to 30%)	50%
PTT	20%	30%

Table 3-8: Overview of saving potentials of NREU for fermentation products from maize starch, relative to their petrochemical equivalents

Land use is an important independent indicator next to non-renewable energy use (see also discussion about the various indicators in Section 3.4.2). Figure 3-17 provides an overview of the requirements of agricultural land per tonne of bio-based chemical. The low and high values represent the extremes minimum and the maximum of all process schemes analysed, while the medium value was calculated as arithmetic mean. The spread between low and high values is rather small (less than ±25%) for eleven of the 15 products. This reflects the fact that the scope to improve the fermentation yields beyond the current-state-of-the art is often limited. The average land use of 0.29 ha/t (0.23 – 0.35 ha/t; see bar on the far right) may be useful for first estimations of the land requirements of a bio-based economy. However, given the substantial differences across the products, more accurate calculations on land use must take into account the production volumes of the individual products (this approach will be taken in Chapter 4).

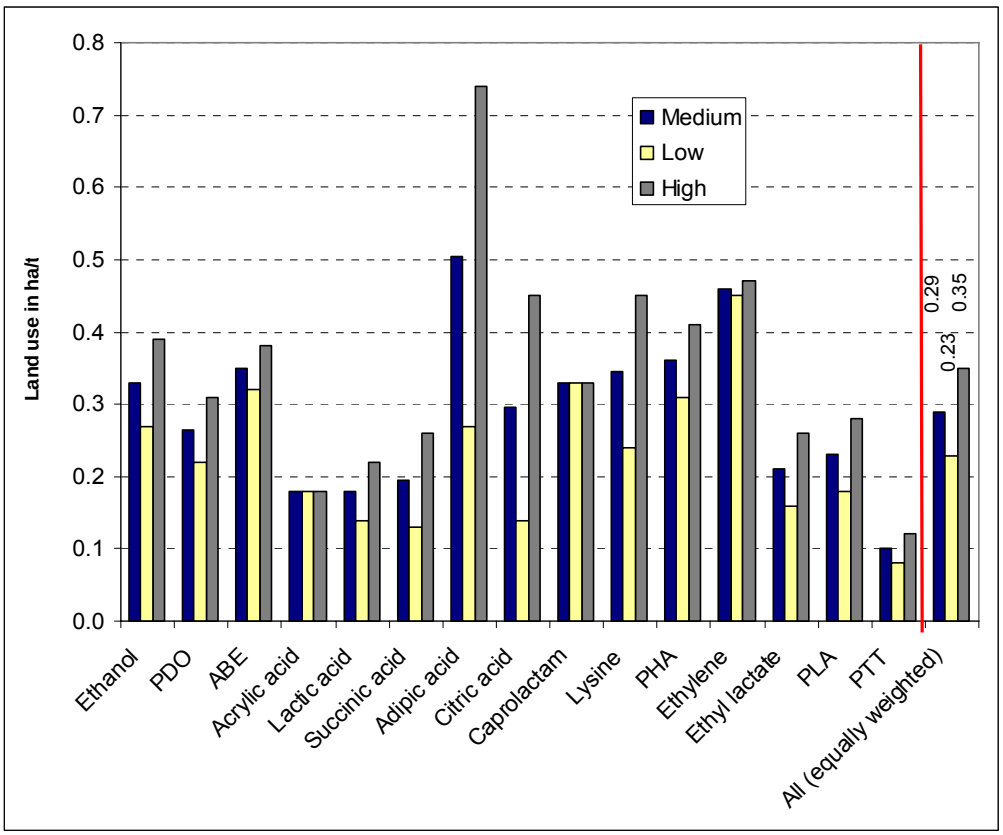

Figure 3-17: Land use per tonne of fermentation products from maize starch

By calculating the arithmetic mean of the energy saving potentials of *all* products shown in Figure 3-16 (for maize starch as feedstock), the *average overall* saving potential can be determined (ideally, the weighted average should be determined but this would require insight into the future production volume for each product concerned). This yields the lower line in Figure 3-18, titled "Overall maize starch". Proceeding likewise for products derived from lignocellulosics and sugar cane gives the other lines in Figure 3-18 (this graph excludes acetic acid and adipic acid because they are clearly unattractive for TODAY; an additional reason for acetic acid is that it remains questionable for the FUTURE; the arithmetic mean also excludes hydrogen because the value is exceptionally high, see earlier explanations; compare Figure 3-16).

One can conclude from Figure 3-18 that starch-derived bio-based chemicals offer saving potentials of NREU compared to the petrochemical benchmark in the range of 30% for TODAY and 50% for the FUTURE. For the switch to lignocellulosics as a feedstock we calculate NREU savings for the FUTURE of 75% compared to the production of petrochemicals nowadays, whereas a switch to sugar cane as feedstock would result in NREU savings of 80% TODAY and nearly 100% in the FUTURE (again with the current production of petrochemicals as benchmark). Note that switching to lignocellulosics feedstocks today is not possible technologically, therefore no value is given here. The ranges in Figure 3-18

represent the maximum and minimum for the individual products (extreme values),[65] while the weighted average of the uncertainties of all products would be clearly lower. For the FUTURE, the ranges in Figure 3-18 are 30%-70% for maize starch, 40%-100% for lignocellulosics and 50%-150% for sugar cane as feedstocks. Values above 100% are due to the fact that some product routes are net producers of energy when based on sugar cane.

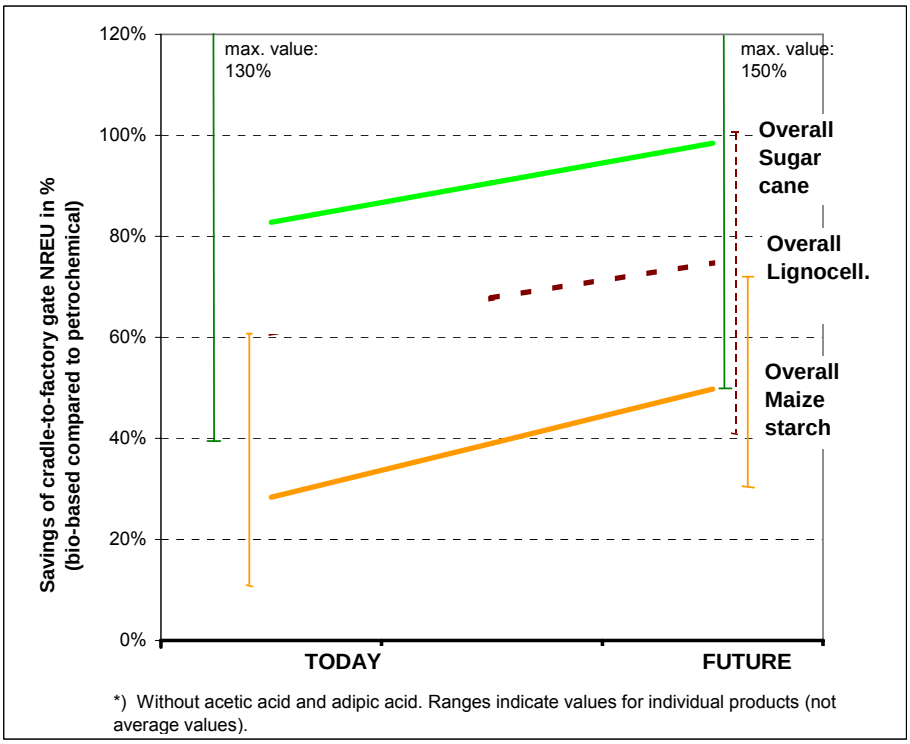

Figure 3-18: Average saving potentials of cradle-to-factory gate NREU for the fermentation products studied

As explained in Section 3.4.2 it is important to simultaneously analyze NREU and land use in addition to the separate analyses discussed above because the two parametres *may* be interrelated for a given process. For simultaneous analysis, the ratio of saved NREU (compared to the production of petrochemicals) and the land requirements can be determined. This indicator quantifies how much energy can be saved per hectare of land and thus helps to assess the environmental attractiveness. As shown in Figure 3-19 the range of values is very large. Around one third of all processes depicted (only processes which *save* NREU compared to their petrochemical equivalents are plotted) allow NREU savings in the range of 80 GJ/ha to 140 GJ/ha/a (110 ± 30 GJ/ha); this is close to the specific yield of producing bioenergy from 1 ha of land cultivated with poplar by co-combustion in a coal-fired power plant.[66] The arithmetic mean of all processes depicted in Figure 3-14 is around 115 GJ/ha/a, i.e. very similar to the value for co-combustion of poplar in a coal-fired power plant (110 GJ/ha/). Around 25% of the depicted cases are above the threshold of 110 GJ/ha/a, some of them substantially. A limited number of processes (approx. 5%) is around or above the level of

[65] For example, for TODAY's fermentation processes based on maize starch, ABE offers savings of 10% only while Ethanol allows to save 60%. The range of 10% to 60% is depicted in Figure 3-18.

[66] The assumed yield of poplar, its heating value and the estimated requirements of non-renewable energy are given in Section 3.4.2 (see text).

230 GJ/ha/a,[67] which represents an estimate of the maximum NREU savings by use of miscanthus as bioenergy. The value for miscanthus can be seen as the highest possible value achievable with bioenergy in Europe because miscanthus has outstandingly high yields under suitable conditions, which are, however, are not a given throughout Europe.
As discussed in the context of Figure 3-14 co-combustion of biomass in a coal-fired power plant allows larger primary energy savings per unit of agricultural land than ethanol production for fuel purposes (see gedged area in Figure 3-19). Fuel ethanol offers NREU saving potentials of 20-30 GJ/ha/a which is by far less than the overwhelming majority of the processes depicted in Figure 3-19.
We can conclude from Figure 3-14 and Figure 3-19 that it cannot be taken for granted that a White Biotechnology process that saves NREU compared to its petrochemical equivalent (in GJ NREU per tonne of product) is also clearly attractive in terms of NREU savings per land use, if compared to bioenergy. At the same time, there are exceptionally attractive options which outpace the possibilities of bioenergy (in terms of NREU savings per land use). This is especially the case for certain processes for succinic acid; other advantageous options are available for PDO and PTT and – with some distance – also for PLA and ABE.

While we have so far used the two bioenergy options as benchmark for maize starch-based chemicals (Figure 3-19), the comparison could also be made with bio-based chemicals derived from lignocellulosics or from sugar cane. The latter, i.e. the comparison of bio-based chemicals from sugar cane with bioenergy would, however, require to extend the portfolio of bioenergy options by the possibilities available in tropical countries. Since the main focus of this study is on Europe, we limit ourselves to the comparison of bio-based chemicals derived from lignocellulosics with bioenergy from poplar and miscanthus. We therefore performed the analysis shown in Figure 3-19 also for chemicals derived from poplar and from miscanthus. The results are as follows:

- The average mean of the NREU savings per unit of land that are achievable with chemicals from poplar has been calculated to be 130 GJ/ha/a. One could argue that only future processes for chemicals production should be taken into account because also the production of fermentable sugar from lignocellulosics is not yet commercially available. Limiting the calculation to the processes estimated with the Generic Approach for the FUTURE gives an average mean of 180 GJ/ha/a. These two results are somewhat higher to higher than the estimate for short rotation poplar as energy crop (110 GJ/ha/a). The choice of poplar as lignocellulosic feedstock for chemicals hence does not change our conclusions presented above. Comparing the results on a product-per-product basis (the results are not presented here in tabular form) we also confirm our earlier conclusion that there are exceptionally attractive options which outpace the possibilities of bioenergy (in terms of NREU savings per land use).
- The average mean of the NREU savings per unit of land that are achievable with chemicals from miscanthus has been calculated to be 190 GJ/ha/a for all processes and 240 GJ/ha/a for FUTURE processes. These two results are rather close to the estimate for miscanthus as energy crop (230 GJ/ha/a), but somewhat on the lower side. The product-by-product comparison leads to the same conclusion as for poplar.

To conclude, the calculations indicate somewhat higher average NREU saving opportunities per unit of land compared to bioenergy for starch-based chemicals and for poplar, while they tend to be somewhat lower for for miscanthus. The comparison on a product-by-product basis leads to the conclusion that, for a few chemicals, the NREU saving possibilities per unit of land are clearly more attractive for bio-based chemicals than for bioenergy.

[67] The assumed yield of miscanthus, its heating value and the estimated requirements of non-renewable energy are given in Section 3.4.2 (see text).

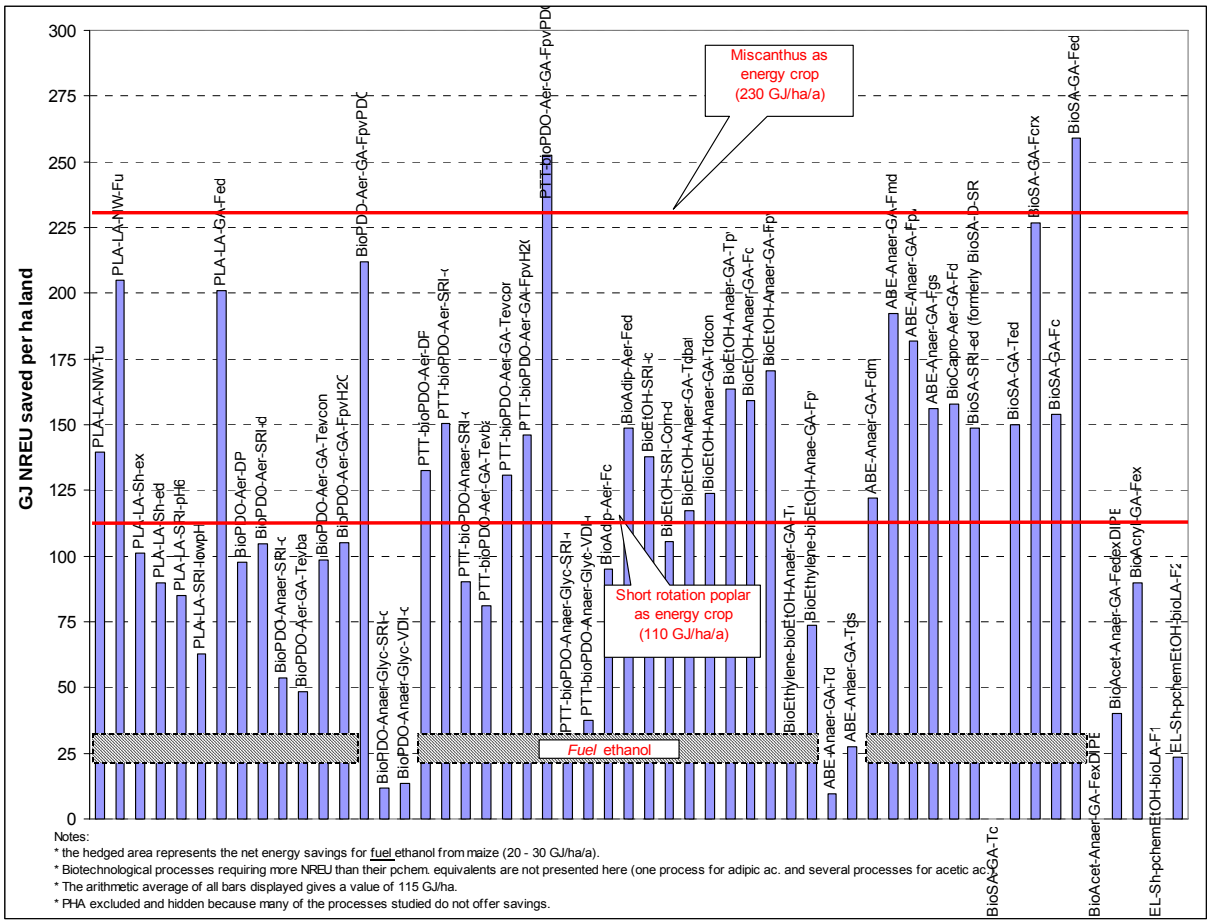

Figure 3-19: Land use efficiency in terms of NREU savings for fermentation products from maize starch - Ratio of savings of non-renewable energy use (NREU savings compared to the petrochemical product) to land used for providing the feedstock for the bio-based product

3.4.4 Overview of the economic results for all fermentation products

As explained in Section 3.4.2 at the example of 1,3-propanediol (PDO), the economic analyses were performed for four price levels for fermentable sugar (70 €/t, 135 €/t, 200 €/t and 400 €/t). The prices for all other inputs were kept constant at present-day values for the calculations presented in this Section 3.4.4 (in contrast to Chapter 4 where, in addition, different levels of fossil fuel prices were considered). The calculation results given in Table 3-9 are presented in graphical form in Figure 3-20 (all calculations were performed with the method explained in Section 3.3.1). In Figure 3-20, the curves give the results of the calculations for bio-based products, while the horizontal lines represent the product value and the market price of the respective petrochemical product. In cases where a petrochemical benchmark does not exist (neither an identical petrochemical product nor a non-identical petrochemical equivalent), only the market price is given (lactic acid, lysine, citric acid). For all bio-based products for which more than one process scheme was calculated two or three curves are shown indicating the overall range of values.

For some products, we find a large difference between the product value of the petrochemical product and the market price. For explanation, we distinguish two cases:

- The market price is substantially higher than the product value of the petrochemical product if the product is a speciality that is currently serving a niche market. This, for example, is the case for ethyl lactate and for PDO (see Figure 3-20). The reasons are the production in relatively small facilities nowadays, the use of these compounds for higher value applications and the imperfect market conditions (very small number of producers). These boundary conditions represent a good starting point for both new producers of bio-based and of petrochemical ethyl lactate and PDO. It is therefore decisive whether the product value is lower for the bio-based product or for the petrochemical product.
- The market price can be clearly lower than the product value if the chemical is commonly produced from petrochemical feedstocks (mature petrochemical product) and if the market conditions are unfavourable. This seems, for example, to be the case for ethylene, acrylic acid and caprolactam (see Figure 3-20). This situation may be the consequence of fierce competition among producers and/or a general economic downturn. Under these conditions the producers have very low or no profit margins and they may not recoup their capital. This may be an acceptable situation for a limited period of time (especially if the production facilities are depreciated). Since it is, however, not acceptable for the longer term the product value of the bio-based product should be compared to the product value of the petrochemical product instead of the market price.

We conclude that – while market prices can act as additional incentive (first case) or as additional obstacle (second case) – conclusions about the economics should be drawn by comparing the product value of the bio-based product with the product value of the petrochemical. The use of the market prices of petrochemicals may, however, be justifiable if the market inequilibrium can be expected to persist or if a “snapshot” of the current situation is supposed to be depicted.

		Production system	Product value **for sugar @ 70EUR/t**	Product value for sugar @ **135EUR/t**	Product value **for sugar @ 200EUR/t**
			(EUR/t)	(EUR/t)	(EUR/t)
Alcohols	Ethanol	BioEtOH-SRI-Td	508	655	803
		BioEtOH-SRI-Corn-Td [1)]	1284	1284	1284
		BioEtOH-Anaer-GA-Tdcont	482	636	791
		BioEtOH-Anaer-GA-Fd	353	502	650
		BioEtOH-Anaer-GA-Fpv	372	521	669
		BioEtOH-SRI-Stover-Td [2)]	n/a	775	n/a
		PchemEtOH *)	900	900	900
		PchemEtOH **)	442	442	442
	PDO	BioPDO-Anaer-SRI-Tdcont	1049	1195	1340
		BioPDO-Aer-SRI-Tdcont	955	1073	1190
		BioPDO-Aer-DP-Tu	897	1053	1208
		BioPDO-Aer-GA-Tevbat	823	991	1158
		BioPDO-Aer-GA-Tevcont	663	831	998
		BioPDO-Aer-GA-FpvH2O	595	726	858
		BioPDO-Aer-GA-FpvPDO	465	597	729
		BioPDO-Anaer-Glyc-SRI-Tdcont [3)]	2689	2689	2689
		BioPDO-Anaer-Glyc-VDI-Tdbat [3)]	2052	2052	2052
		PchemPDO-Propyl-DP *)	1203	1203	1203
		PchemPDO-EO-SRI *)	1124	1124	1124
		PchemPDO-Acro-SRI *)	2995	2995	2995
		PchemPDO **)	2414	2414	2414
	ABE	BioABE-Anaer-GA-Tdcont	1225	1430	1635
		BioABE-Anaer-GA-Tgscont	1164	1369	1574
		BioABE-Anaer-GA-Fdm	484	656	829
		BioABE-Anaer-GA-Fmd	440	612	785
		BioABE-Anaer-GA-Fpv	393	565	737
		BioABE-Anaer-GA-Fgs	394	566	739
		PchemBut-PropylRh *)	747	747	747
		PchemButanol **)	500	500	500
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	2082	2222	2361
		BioAcet-Anaer-GA-Ted	2069	2208	2346
		BioAcet-Anaer-GA-FexTOPO	729	806	882
		BioAcet-Anaer-GA-FexDIPE	620	698	776
		BioAcet-Anaer-GA-FedexDIPE	745	822	899
		BioAcet-Anaer-GA-Fed	672	749	826
		PchemAceticAcid **)	400	400	400
	Acrylic acid	BioAcryl-Anaer-GA-Fex	956	1052	1148
		PchemAcryl-Propyl *)	1031	1031	1031
		PchemAcrylicAcid **)	880	880	880
	Lactic acid	BioLA-SRI-TpH6	843	922	1001
		BioLA-SRI-FlowpH	775	854	933
		BioLA-NW-Tu	762	842	923
		BioLA-Sh-Fex	693	772	851
		BioLA-Sh-Fed	903	982	1060
		BioLA-Anaer-GA-Fed	385	460	536
		BioLA-NW-Fu	409	485	561
		BioLA **)	1390	1390	1390
	Succinic acid	BioSA-TNO-edc	645	645	645
	Succinic acid	BioSA-Anaer-GA-Tc	867	945	1023
		BioSA-Anaer-GA-Ted	752	830	908
		BioSA-Aer-SRI-Fed	1112	1180	1248
		BioSA-Anaer-GA-Fcrx	470	539	607
		BioSA-Anaer-GA-Fc	528	586	645
		BioSA-Anaer-GA-Fed	570	638	707
		PchemMaleicAnhydride **)	694	694	694
		PchemSA-MalAnhydr	n/a	n/a	n/a
	Adipic acid	BioAdip-Aer-GA-Tc	2579	2977	3375
		BioAdip-Aer-GA-Fc	978	1123	1269
		BioAdip-Aer-GA-Fed	1051	1200	1349
		PchemAdipicAcid **)	1090	1090	1090
	Citric acid	BioCit-Aer-SRI-Tevc [4)]	1519	1519	1519
		BioCit-Aer-SRI-Tix	972	1148	1325
		BioCit-Aer-GA-Tpc	871	1116	1362
		BioCit-Aer-GA-Fc	380	454	528

[1)] The original process data used cover all steps starting with the intake of corn. For this reason, the values in this row are identical.

[2)] The original process data used cover all steps starting with the intake of corn stover at a price of 26 EUR/t. The assignment to the column for a price of 135 EUR/t fermentable sugar is a rough estimate (available data do not allow an

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane). For this reason, the data in this row are identical.

[4)] The original process data used refer to the use of cane molasses. The calculations have been performed assuming a price of 220 EURO/t cane molasses.

*) Calculated product value (for the respective feedstocks such as ethylene and propylene, the market price was used; if this was not available, the product value was calculated.

**) Market price

Table 3-9, Part 1: Product value and Price for bio-based and equivalent petrochemical-based platform chemicals and products

		Production system	Product value **for sugar @ 70EUR/t**	Product value for sugar @ **135EUR/t**	Product value **for sugar @ 200EUR/t**	Product value **for sugar @ 400EUR/t**
			(EUR/t)	(EUR/t)	(EUR/t)	(EUR/t)
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	1201	1379	1557	2104
		PchemCaproButadiene *)	1984	1984	1984	1984
		PchemCapro **)	1320	1320	1320	1320
	Lysine	BioLys-Aer-SRI-Tix	2111	2301	2491	3075
		BioLys-Aer-SRI-Tsp	1227	1448	1670	2351
		BioLys-Aer-GA-Tix	1578	1889	2200	3158
		BioLys-Aer-GA-Fad	803	1022	1241	1915
		BioLys **)	1440	1440	1440	1440
H_2	Hydrogen	BioH2-A&F-gs [1)]	1135	1135	1135	1135
		PchemH2 **)	1616	1616	1616	1616
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	988	1160	1333	1863
		BioPHAmcl-A&F-FA-Oilex [2)]	1865	1865	1865	1865
		BioPHA-GA-Toa	1083	1306	1528	2213
		BioPHA-GA-Th	1543	1761	1978	2648
		BioPHA-GA-Tey	2156	2374	2591	3261
		BioPHA-GA-Tex	1601	1811	2021	2668
		BioPHA-GA-Texey	2218	2428	2638	3284
		BioPHA-GA-OilTexey [2)]	2747	2747	2747	2747
		BioPHBV-SRI-Tey-1	4281	4488	4694	5330
		BioPHB-SRI-Tey-2	3259	3465	3672	4308
		BioPHA-GA-Fey-1	4503	4670	4837	5350
		BioPHA-GA-Fey-2	1087	1254	1421	1934
		PchemHDPE **)	1000	1000	1000	1000
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	1013	1283	1553	2384
		BioEthylene-BioEtOH-Anae-GA-Fpv	821	1081	1340	2138
		PchemEthylene **)	724	724	724	724
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	863	922	981	1161
		EL-Sh-pchemEtOH-bioLA-F2	1287	1346	1404	1585
		BioEL-NW-bioEtOH-bioLA-T1	1075	1206	1337	1740
		BioEL-Sh-bioEtOH-bioLA-F1	833	956	1079	1457
		BioEL-NW-bioEtOH-bioLA-F2	791	916	1040	1423
		BioEL-Sh-bioEtOH-bioLA-F3	1233	1291	1350	1531
		BioEL-Sh-bioEtOH-bioLA-F4	880	1006	1131	1517
		PchemEthylAcetate **)	649	649	649	649
		PchemBenzene **)	401	401	401	401
		PchemEGBE **)	1914	1914	1914	1914
		PchemMEK **)	787	787	787	787
		PchemAcetone **)	417	417	417	417
	PLA	BioPLA-bioLA-SRI-TpH6	1383	1484	1585	1896
		BioPLA-bioLA-SRI-FlowpH	1423	1524	1625	1935
		BioPLA-bioLA-NW-Tu	1307	1410	1513	1830
		BioPLA-bioLA-Sh-Fex	1337	1438	1539	1850
		BioPLA-bioLA-Sh-Fed	1327	1428	1529	1840
		BioPLA-bioLA-Anaer-GA-Fed	1282	1379	1476	1773
		BioPLA-bioLA-NW-Fu	1176	1274	1371	1672
		PchemPET Amorph **)	1200	1200	1200	1200
		PchemPolystyrene General Purpose **)	1070	1070	1070	1070
		PchemPE LD **)	1000	1000	1000	1000
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	1111	1157	1203	1344
		PTT-bioPDO-Anaer-SRI-Tdcont	1148	1205	1262	1437
		PTT-bioPDO-Aer-DP-Tu	1088	1149	1210	1398
		PTT-bioPDO-Aer-GA-Tevbat	1059	1125	1191	1392
		PTT-bioPDO-Aer-GA-Tevcont	997	1062	1128	1330
		PTT-bioPDO-Aer-GA-FpvH2O	970	1021	1073	1231
		PTT-bioPDO-Aer-GA-FpvPDO	919	971	1022	1181
		PTT-bioPDO-Anaer-Glyc-SRI-Tdcont [3)]	1790	1790	1790	1790
		PTT-bioPDO-Anaer-Glyc-VDI-Tdbat [3)]	1541	1541	1541	1541
		PTT-PchemPDO-Propyl-DP *)	1712	1712	1712	1712
		PTT-PchemPDO-EO-SRI *)	1177	1177	1177	1177
		PTT-PchemPDO-EO-Shell	n/a	n/a	n/a	n/a
		PTT-PchemPDO-Acro-SRI *)	1910	1910	1910	1910
		PchemPET Amorph **)	1200	1200	1200	1200
		PchemNylon-6	3228	3228	3228	3228
		PchemNylon-6,6	3402	3402	3402	3402

[1)] The original process data used refer to the use of potato slurry proteins and potato steam peals. The total price of these two feedstocks is assumed to be zero. For this reason, the values in this row are identical.

[2)] This process uses fatty acids (FA) as feedstock, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil. The calculations have been performed assuming a price of rapeseed crude oil of 500 EURO/t. The results are reported in the column for maize starch. For this reason the values in this row are identical.

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics and sugar cane). For this reason the values in this row are identical.

*) Calculated product value (for the respective feedstocks such as ethylene and propylene, the market price was used; if this was not available, the product value was calculated.

**) Market price

Table 3-9, Part 2: Product value and Price for bio-based and equivalent petrochemical-based platform chemicals and products

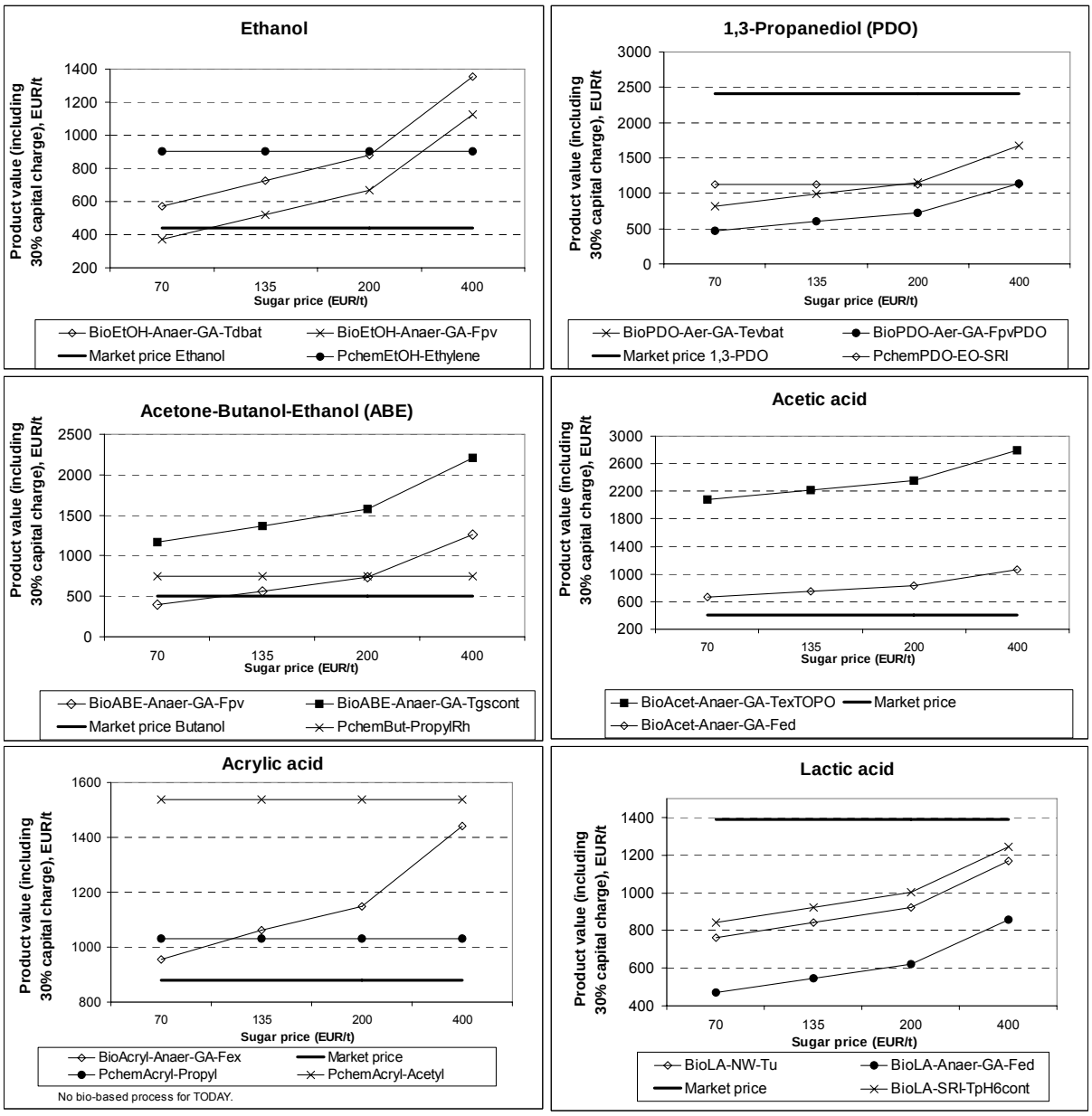

Figure 3-20: Part 1:Economics of the production of bio-based chemicals depending on the sugar price level and on the level of technology ("T" in bioprocess name for TODAY, "F" for FUTURE. All petrochemical processes for TODAY. Important note: the price basis for fossil feedstocks is 25 US$/barrel)

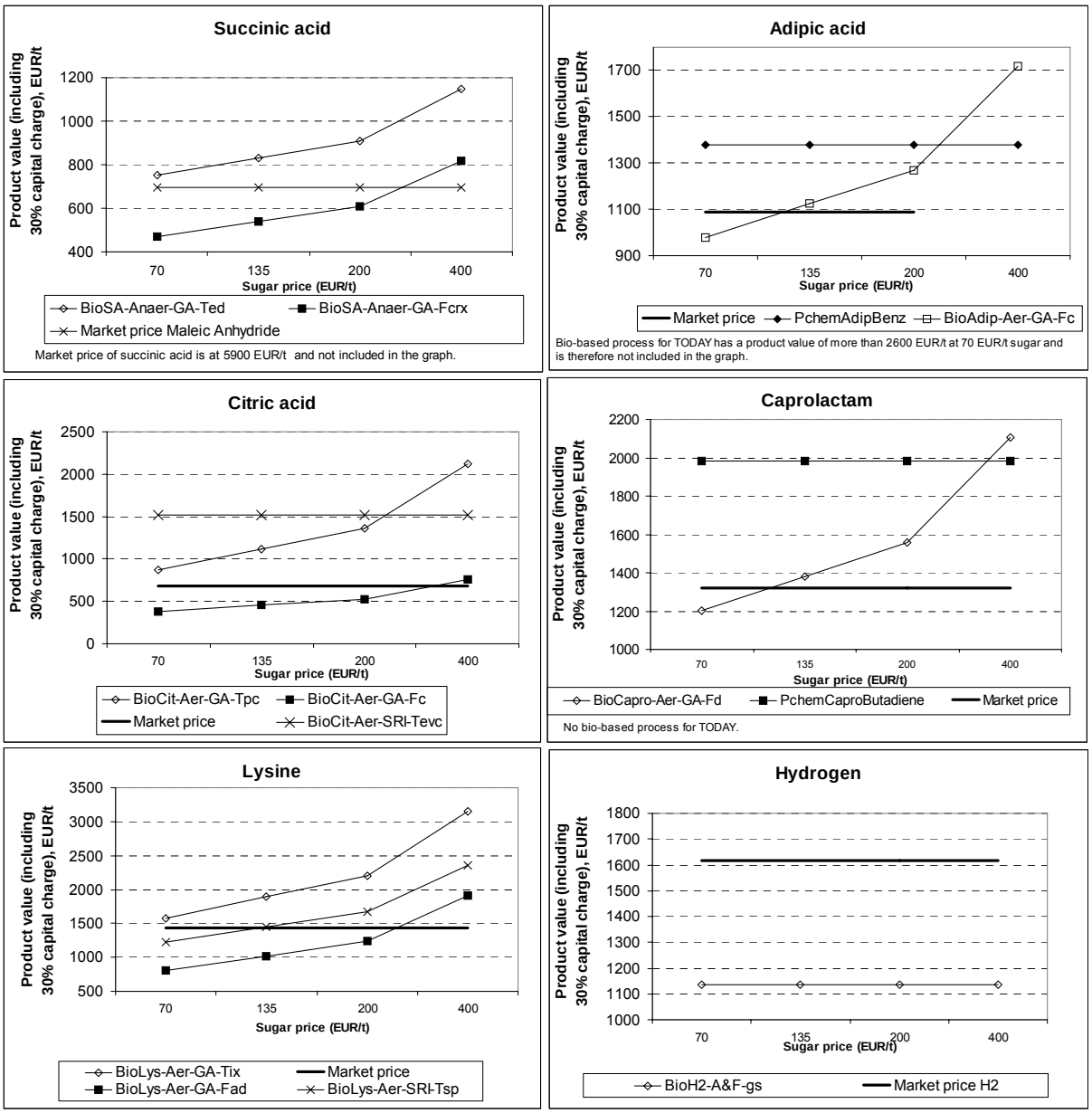

Figure 3-20, Part 2: Economics of the production of bio-based chemicals depending on the sugar price level and on the level of technology
("T" in bioprocess name for TODAY, "F" for FUTURE. All petrochemical processes for TODAY. Important note: the price basis for fossil feedstocks is 25 US$/barrel)

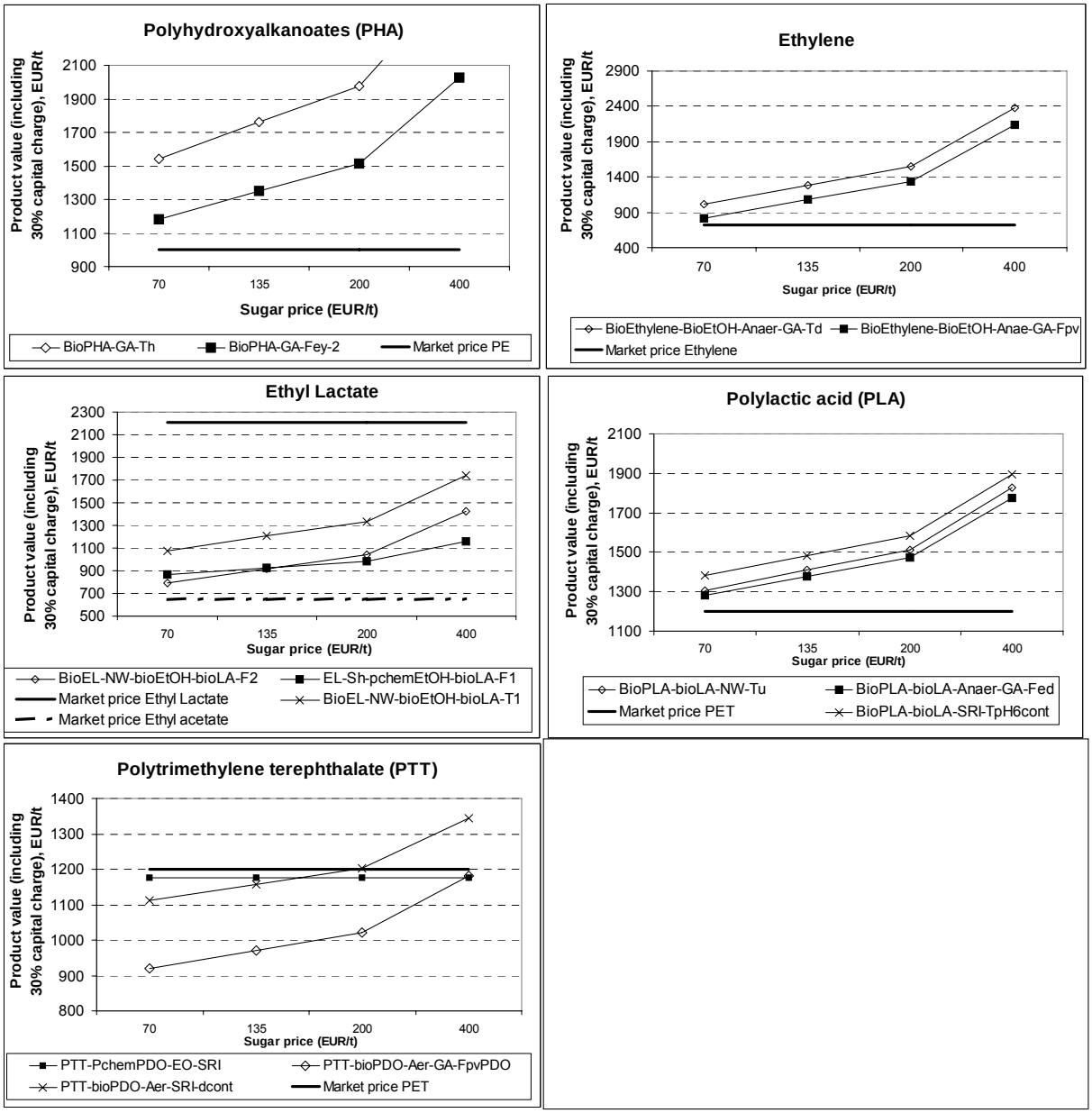

Figure 3-20, Part 3: Economics of the production of bio-based chemicals depending on the sugar price level and on the level of technology
("T" in bioprocess name for TODAY, "F" for FUTURE. All petrochemical processes for TODAY. Important note: the price basis for fossil feedstocks is 25 US$/barrel)

Comparing the product value of the bio-based product with that of the petrochemical product conclusions about the economic viability can be drawn which are shown in Table 3-10. It is very important to realize that this comparison refers to an oil price level of 25 US$/barrel For some petrochemical products, for which the market price differs substantially from the product value of the petrochemical route, indicating an imbalance in the market (e.g., for ethanol; compare Figure 3-20, Part 1). In these cases a judgement had to be made as to whether the bio-based products are competitive or not (in unclear cases the the possibility is

stated in brackets in Table 3-10). For lactic acid, citric acid and lysine, production from petrochemical feedstocks does not exist or is insignificant. These products have therefore not been added to the table in spite of the fact that they are being produced by biotechnological processes in commercial production facilities.. Hydrogen was neither added because only one bio-based process was studied and because it operates on a mixture of feedstocks (potato slurry proteins and potato steam peals) the total cost of which was assumed to be zero.

Sugar price level	Economically viable products	
	TODAY	FUTURE
70 €/t	- Ethanol - PDO - Succinic acid (possibly) - PLA (possibly) - PTT	- Ethanol - PDO - PTT - Butanol (ABE) - Acetic acid (possibly) - Acrylic acid - Succinic acid - Adipic acid - Caprolactam - PHA (possibly) - Ethylene (possibly) - Ethyl acetate (possibly) - PLA (possibly) - PTT
135 €/t	- Ethanol (possibly) - PDO - PTT	- Ethanol - PDO - PTT - Butanol (ABE) - Acrylic acid (possibly) - Succinic acid - Adipic acid (possibly) - Caprolactam (possibly) - PTT
200 €/t	- Ethanol (possibly) - PDO - PTT (possibly)	- Ethanol (possibly) - PDO - Butanol (ABE; possibly) - Succinic acid - Adipic acid (possibly) - Caprolactam (possibly) - PTT
400 €/t		- PDO - Succinic acid (possibly) - PTT (possibly)

No direct comparison was possible for lactic acid because there is no meaningful petrochemical production (only specialties). However, compared to the current market price, all processes leading to lactic acid are economically viable.

Table 3-10: Economic viability of fermentation products as a function of the price level of fermentable sugar and depending on the technology level for White Biotechnology (Important note: the price basis for fossil feedstocks is 25 US$/barrel)

All calculation results presented so far refer to a plant size of 100 kt p.a. Sensitivity analyses have been performed to assess the influence of scale on the economics of bio-based prosucts studied. The calculations were performed for butanol (ABE process), ethanol, PDO, acrylic acid, acetic acid, lactic acid, adipic acid, succinic acidcaprolactam and PHA. The assumed plant sizes range between 200 kt and 400 kt and are given in Table 3-2. According to our calculations, the larger scale reduces the product value (production costs) in most cases by

around 10% (in cases of low sensitivity around 5% and and for high sensitivity max. 20%). The comparison of these results with the values for a 100 kt plant as displayed in Figure 3-20 shows that scale has practically no influence on the competitiveness of the bio-based process relative to its petrochemical equivalent, i.e. the results presented above are in general robust to scale. Mostly, the values found for larger scale are still within the range of values shown in Figure 3-20 for various processes. Only in exceptional cases larger scale leads to a different conclusion by making the bio-based process more attractive (according our calculations this could occur for caprolactam).

The results given in Table 3-10 and Figure 3-20 are subject to uncertainty due to the numerous assumptions and input data, which they are based on. Since this may be particularly relevant for the assumptions made for future processes with regard to concentration, productivity and yield (see Chapter 3.1.1, Table 3-2) we discuss the influence of these parameters in Box 3-3. Moreover, for example, process integration (e.g., the combination of starch production and processing with fermentation) may allow better economic viability than reflected by our calculations. Also the opposite is possible. It should be borne in mind that all calculations in Chapter 3 have been made assuming a crude oil price level of US$ 25/barrel (and 4 €/GJ for final users of natural gas in the chemical industry). In the context of our scenario analyses in Chapter 4 we will now take into account the effect of higher oil (and other fossil fuel) prices.

We conclude that a rather limited number of products is economically attractive TODAY under sugar price levels as they are currently prevailing in Europe and in the U.S. As a consequence of improved technology in the FUTURE, the number of economically attractive products increases decisively. In order to make clearly more products attractive from an economic point of view, lower sugar prices would hence be required in addition to substantial progress in industrial biotechnology and downstream processing (valid for a price level of US$ 25/barrel crude oil).

As pointed out in Chapter 3.1.1, the data for concentration, productivity and yield given in Table 3-2 have a large influence on the final outcome of the environmental and the economic assessment. For a few products (especially 1,3 propanediol and lactic acid) it has been possible to compare the calculation results for TODAY performed with the Generic Approach with company data from pilot plant or industrial facilities (these data were provided by BREW partners). According to this comparison (for energy use) the calculations according to the Generic Approach reflect well the current processes (compare below Section 3.4.2, 3.4.3 and Appendix A8 - A10). However, it should be kept in mind that only very few of these comparisons could be made for TODAY and no such basis for comparison exists for the FUTURE. For the datasets assumed for the FUTURE, an attempt was made to ensure internal consistency of the values across the products, thus reflecting a comparable level of ambition for the production of all products by means of FUTURE technology. However, this is a very difficult task and other experts may consider some data for the FUTURE in Table 3-2 to be too ambitious or too conservative. For example, some experts may find the assumption made for FUTURE concentrations to be too low for continuous fermentation designs while the assumptions for FUTURE yields and especially for FUTURE productivity might be considered by some to be too optimistic. For example, for ethanol, the current productivity is around 2.2 g/l/h, while FUTURE productivity has been assumed to be 50 g/l/h (see Table 3-2; the results given in Tables 3-7 to 3-10, Figure 3-14 to 3-20 and in Chapter 4 for FUTURE technology are based on this value). The views about the maximum feasible values differ:

While in Ullmann's Encyclopedia several authors are quoted reporting values of 30 g/l/h to 50 g/l/h and some publications are referred to reporting values lying even between 50 g/l/h and 100 g/l/h (Kosaric, et al., 1997), engineering companies building ethanol plants consider a value of 2.2 g/l/h as maximum for TODAY if starch is used and 4-8 g/l/h if the plant is operated on sugar cane (with cell recycle; pers. communication Vogelbusch, Austria, 2006). Sugar cane-based processes in the FUTURE are expected to reach up to around 10 g/l/h (Vogelbusch, Austria, 2006). This higher value could, in principle, be achieved also with starch if saccharification could be realized in a separate, preceding step. Productivities of nearly 30 g/l/h can already be achieved nowadays if a conversion degree for fermentable sugar of only 80% is accepted, i.e. for a loss of sugar of 20% (pers. communication, CTC, 2006); however; engineering problems related to the release of large amounts of heat and foaming raise the question whether values in this order of magnitude (as assumed in BREW also for other processes) are at all desirable.

In order to assess the influence of the productivity values assumed for the FUTURE, a sensitivity analysis was performed for ethanol. As shown in the table below the difference between a productivity of 10 g/l/h and 50 g/l/h on investment, primary energy and product value (production costs plus profits) is less than 5%. This demonstrates that, for ethanol, the sensitivity to marginal improvements decreases beyond a threshold value of around 10 g/l/h. Substantially lower productivities than those used in the BREW calculations (see Table 3-2) would therefore most likely lead to the same result. For ethanol, the productivities could be lowered by a factor of 5 without changing the overall findings (10 g/l/h instead of 50 g/l/h instead). Further investigations would be required in order to understand the level of the threshold values for *all* products investigated in the BREW study. While this type of analyses is beyond the scope of the BREW project they would be useful in order to formulate quantitative R&D goals.

		Produc-tivity (g/l/h)	Concen-tration (g/l)	Invest-ment (mill. EUR)	Power (GJ/t) *)	Steam (GJ/t) *)	Primary energy (GJ/t) **)	Product value (EUR/t)	
								70 EUR/ t sugar	400 EUR/ t sugar
Evap Dist	**TODAY**	2.2	100	61.0	1.2	3.7	12.5	482	1266
EvapDist	**FUTURE, low productivity**	10	130	40.7	0.5	3.1	9.2	366	1120
EvapDist	**FUTURE, chosen value**	50	130	37.7	0.4	3.1	8.8	353	1106

Scale (for all calculations): 100 kt p.a.

*) System boundaries: Upstream = Input of glucose; Downstream = Output of ethanol

**) Final energy has been converted to primary energy assuming an weighted efficiency of 39.6% for the conversion of fossil fuels to power (according to Table A2.4, see Appendix 2; value accounts for both power generation within the chemical sector and for the public grid) and 2.73 GJ primary energy per tonne of steam (according to Table A2.5, see appendix).

Box 3-3: Sensitivity of the final results to the assumed values for productivity

3.4.5 Energy analysis and techno-economic assessment for enzymatic conversions

Generally speaking, the advantages of enzymatic processes are that the selectivities are higher and that less undesired byproducts are formed compared to conventional processes. As a consequence, the process schemes are often simpler for enzymatic processes compared to conventional processes, hence entailing lower investment costs. In addition, temperatures and pressures are, in general, lower for enzymatic processes. In this chapter we present the techno-economic analysis of four products which can either be produced enzymatically or by conventional processes. The four products are fatty acids, oleyl oleate, glycerol monooleate and adipic acid.

Fatty acids

In Europe, the annual production of fatty acids is nowadays around of 1.4 million tonnes (Poulina 2005). Fatty acids are used for the production of fatty alcohols, esters, amides, amines, nitriles and soaps. These products and their derivatives are used in a variety of applications including surfactants for detergent use, emulsifiers, thickeners, adhesives, corrosion inhibitors, fabric softeners and flotation agents (Weissermel and Arpe 2003). Fatty acids are produced by splitting of fats and oils such as rape oil, soya oil and tallow. Conventional splitting, as nowadays applied, is performed with water at elevated temperature and requires no catalyst or auxiliary.[68] Enzymatic splitting could be an option for the future and involves the use of an enzyme that acts as (bio-)catalyst. Both processes, the conventional and the enzymatic, have practically identical yields and lead both to about 10% of glycerol which is formed as byproduct. In the enzymatic process a more concentrated acquoeus solution of glycerol is formed compared to the conventional process.

For our techno-economic process, we compare an enzymatic and a conventional process which both have a capacity of 150 kt p.a. As shown in Figure 3-21, the renewable energy use (REU) is identical in the two cases because renewable energy is only supplied to the process in the form of feedstocks (fats and oils) and because the yields are practically identical. The non-renewable energy (NREU) is clearly lower and originates from the use of process energy in the form of steam and power and by *indirect* energy use which is related to auxiliaries (here, in particular, the enzyme). In the default cases, the NREU is practically identical for the conventional and the enzymatic process. The error bar in Figure 3-21 is the consequence of the uncertainty about the energy use related to enzyme production. Information on energy use and the environmental impacts of enzyme production is very scarce. As shown in Table 3-11, non-renewable energy use for enzyme production can differ by around a factor of 10 depending on the enzyme even if the processes have been optimized over decades and if gene-modified microorganisms are used. Without optimization, the range of NREU requirements can be much higher than those reported in Table 3-11. According to analyses performed by novozymes for a selected enzyme product, the NREU and other environmental impacts are up to a factor of 6 larger than in the optimized case; in combination with the data in Table 3-11 this would yield NREU values of up to 750 MJ. Even much higher values have been found in few other sources (see Table A1.3 in the Appendix). Enzyme application at the large scale

[68] Fats and oils are triglycerides which fall under the chemical group of esters. Splitting of the ester linkage with water allows the isolation and purification of the fatty acid.

requires the use of optimized enzyme production systems and we therefore use the data in Table 3-11 as basis (we proceed likewise also for the other products, see below). Since the energy required to produce the type of enzymes needed for enzymatic splitting of fats and oils is unknown, we assumed in Figure 3-21 the arithmetic mean of the values given in Table 3-11, i.e. 70 MJ/kg enzyme and 5.7 kg CO_2,eq/kg enzyme (in both cases ±80%). he Even a larger uncertainty range for enzyme production than that reflected by the error bar in Figure 3-21 is unlikely to change the conclusion from the comparative analysis (Figure 3-21). The reason is that the level of NREU is already very low which becomes clear by comparison with other chemical products: While, according to the cases shown in Figure 3-21, 3 to 4 GJ NREU (cradle-to-factory gate) are required per tonne of fatty acid, typical NREU values for chemical intermediates without feedstock are between 15 and 30 GJ/t (cradle-to-factory gate); for petrochemical products, the fossil feedstock needs to be added, resulting in typical overall values between 40 and 70 GJ/t (cradle-to-factory gate; Patel 2003). The overall level of NREU is hence at least by a factor of 10 lower in enzymatic processes (using a petrochemical feedstock) compared to a petrochemical intermediates. It can be concluded that, for fatty acids, the *overall* potential for saving energy and reducing related environmental impacts by shifting from the conventional process to an enzymatic process is most likely negligible.

Nevertheless it is of interest for industrial producers to shift to the enzymatic process if the economics are attractive. According to our analysis the high enzyme cost are currently prohibitive for the application of the enzymatic process; if implemented today, enzyme cost would account for around three quarters of the total production cost (product value). If, in future, enzyme prices drop to around 10 or tens of Euros per kg of enzyme, then enzymatic processes could become competitive. The economic viability will then depend on a variety of further conditions, e.g., which price can be fetched for glycerol as a function of its concentration and whether waste heat for water removal from glycerol is available on site and at which price.

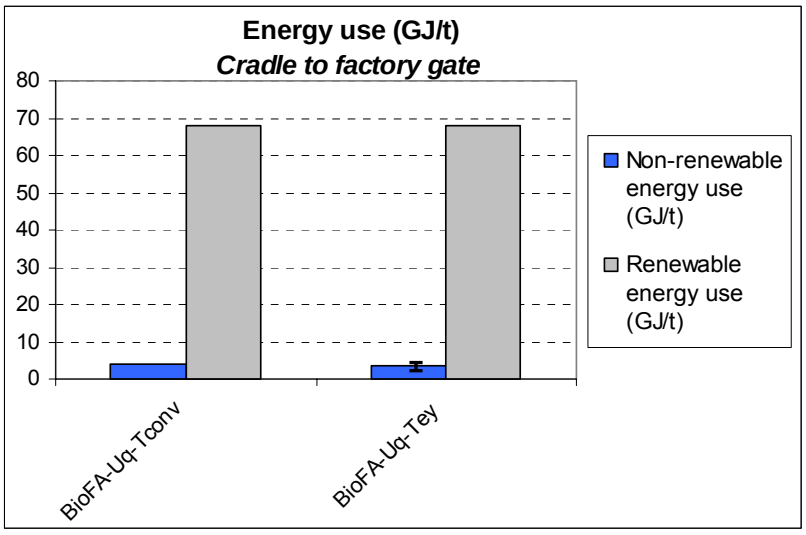

Figure 3-21: Non-renewable energy use for fatty acid production using conventional splitting and enzymatic splitting

	Very low (Gene-modified)	Good (Gene-modified)
NREU ($MJ_{prim.}$/kg)	15	125
NRGHG (kg CO_2eq./kg)	1.2	10.2

Table 3-11: Estimated non-renewable energy use (NREU) and non-renewable greenhouse gas emissions (NRGHG) for enzyme production (preliminary estimates by novozymes, pers. comm., 2006)

Oleyl oleate

Oleyl oleate, a biolubricant, is produced by esterification of oleic alcohol and oleic acid by use of *p*-toluene-sulfonic acid as conventional catalyst or, alternatively, with lipases employed as biocatalysts. The catalyst requirements, the reaction conditions and the features of the process scheme for product separation and purification are given in Table 3-12. The conversion rates are very high in all cases (clearly beyond 99%). However, the conventional esterification process forms more byproducts compared to the enzymatic process, hence requiring additional workup and leading to additional product losses; as a consequence, the *end* product yield may be around 10% lower for the conventional process compared to the enzymatic process.

As shown in Table 3-12 the reaction conditions (temperature, pressure) are milder for the enzymatic process compared to the conventional process. At the same time it needs to be taken into account that the process conditions are already very mild for the conventional process. Considering also the possibilities of heat integration, the *direct* energy requirements can be considered to be roughly identical in the two cases. *Indirect* energy use (and other environmental impacts) due to the use of the raw materials and auxiliaries are considered separately. While the *indirect* energy use related to raw material use (feedstock) cancels out (because the yields are roughly identical), this may not be the case for the catalysts used. We have estimated the NREU of *p*-toluene-sulfonic acid (catalyst for the conventional process) to be around 40 GJ/t of enzyme which is within the range of estimates for enzyme production (compare Table 3-11). While future technological progress my reduce the energy use for enzyme production towards the lower values in Table 3-11, the energy savings are likely to be small, given the fact that the conventional process already requires only very little energy. In line with the outcome of the analysis for fatty acids, we conclude that, for olely oleate, the *overall* potential for saving energy and reducing related environmental impacts by replacing the conventional process by a biocatalytic process is marginal. .

Process type	Reactor type	Catalyst type	Catalyst quantity (t/t oleyl oleate)	Reaction conditions	Downstream processing	Refining
Conventional	Stirred tank (batch)	*p*-toluene-sulfonic acid (TSA)	0.006	- 130 °C - Atmosph. pressure	1. Neutralization 2. Washing 3. Centrifugation	1. Bleaching 2. Deodorization 3. Drying
Enzymatic	Stirred tank (batch)	Immobilized lipase	0.001	- 60 °C - 100 mbar	1. Filtratation 2. Enzyme recovery	1. Deodorization 2. Drying
	Fixed bed (batch)	Immobilized lipase	0.0002	- 60 °C - Atmosph. pressure	1. Flash distillation	1. Deodorization 2. Drying

Table 3-12: Process parameters for the conventional and the enzymatic production of oleyl oleate (Vicente, M.; Aracil, J.; Martinez, M., 2005a; data on catalyst use originate from industry sources; according to other industry sources the catalyst use could be as low as 0.0005 kg enzyme/kg product)

While we did not find energy use and the related environmental impacts to be strong drivers for a process change, the situation could be different for economics. In our analysis of production cost we study two plant sizes, with scales of 10kt and of 100 kt. While we have estimated the investment cost of a conventional plant with an annual capacity of 10 kt at 15 million €, the investment cost of both enzymatic processes (stirred tank and fixed bed) have been estimated at 10 million €. At a 30% capital charge (see Chapter 3.3) the resulting savings in capital expenditures of 5 million € translate to an advantage for the enzymatic processes of 150 €/t oleyl oleate. This advantage is a consequence of the simpler process scheme for the enzymatic processes (which we did not find in the case of fatty acids, see above). Energy costs (*direct* energy use) can be assumed to be very similar for all three process schemes. Moreover, the cost of *p*-toluene-sulfonic (and many other conventional catalysts) is practically negligible (estimated at 1.6 €/t oleyl oleate). We therefore conclude that the enzymatic process is economically advantageous if enzyme costs are below 150 €/ton oleyl oleate. For a plant with an annual capacity of 100 kt, the analogous calculation leads to a breakeven enzyme cost of 50 €/ton oleyl oleate. Given an enzyme use of 0.001 t/t oleyl oleate in the case of the stirred tank (Table 3-12) this translates to a breakeven enzyme price of 150 €/kg for the 10 kt p.a. plant and of 50 €/kg for the 100 kt p.a. plant. The respective values for the fixed bed process with an enzyme use of 0.0002 t/t (Table 3-12) are enzyme prices of 750 €/kg for the 10 kt p.a. plant and of 250 €/kg for the 100 kt p.a. plant. These results are represented in Figure 3-22 by the points that are connected with diagonal, broken lines. The horizontal lines represent current market prices for enzymes. Points below the horizontal lines represent cases that are economically viable.

Since enzymes are taylored to the respective purpose, prices can range considerably. The real enzyme cost is likely to lie between the values given in Figure 3-22 for Lipozyme RM IM and Lipozyme TL IM. As a consequence, the enzymatic process is economically less attractive than the conventional process for the stirred tank both for a plant of 10 kt p.a. and 100 kt p.a. If, however, the enzyme cost for the stirred tank could be reduced to that of Lipozyme TL IM, the large-scale process would become economically viable. Analogous reasoning for the stirred tank leads to the conclusion that the 10 kt p.a. plant is already economically viable today, while futher cost reduction would be required to reach this goal also for the large-scale plant. Again, the latter does not seem impossible in view of the large progress that is being made in White Biotechnology in general and enzyme production in particular.

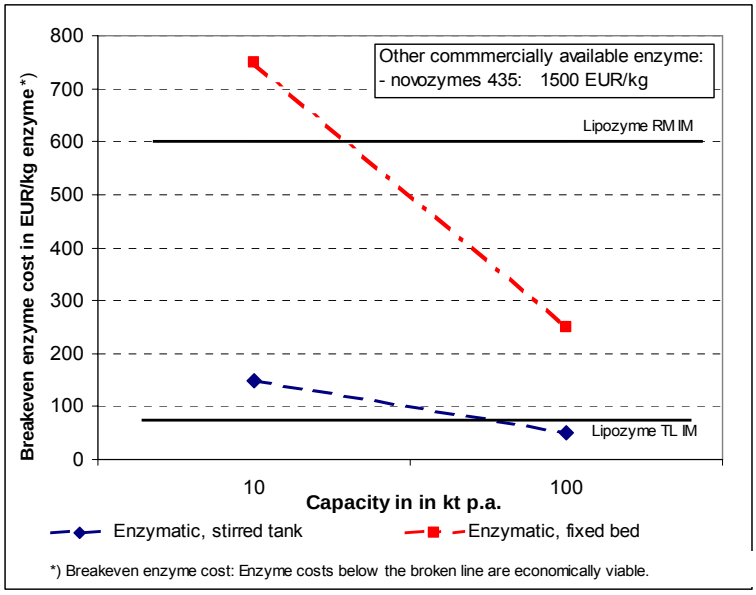

Figure 3-22: Breakeven enzyme cost for oleyl oleate production in different reactor systems

Monoglycerides

Monoglycerides, which are used as biosurfactants, are produced by the reaction of triglycerides with glycerol in transesterification processes. Most of the reasoning and of the conclusions just discussed for oleyl oleate apply also for monoglycerides. As representatives of the group of monoglycerides we discuss briefly the production of glycerol monooleate and of glycerol monoricinolate.

The process features are given in Table 3-13. As for oleyl oleate and for most ester products in general, the conversion rates are very high in all cases, with enzymatic processes having the advantage of producing less undesired byproducts. While the reaction conditions (temperature, pressure; see Table 3-13) are milder for the enzymatic process leading to glycerol monooleate compared to the conventional process, the same reasoning as for oleyl oleate leads to the conclusion that the *direct* energy requirements are roughly identical in the two cases. This excludes *indirect* energy use (and other environmental impacts). The indirect energy use related to raw material use cancels out (because the yields are roughly identical). Regarding the catalysts, we have estimated the NREU of sodium hydroxide (NaOH) at approximately 42 GJ/t which is again within the range of estimates for enzymes (compare Table3-11). As stated in the chapter above for oleyl oleate (3.4.3.1) it can be expected that future technological progress will reduce the energy use for enzyme production towards the lower values in Table 3-11. Nevertheless the energy savings compared to the conventional process are likely to be very small given the fact that the conventional process already requires only very little energy. We conclude that, for glycerol monooleate, the *overall* potential for saving energy and reducing related environmental impacts by shifting from the conventional process to a biocatalytic process is marginal.

Apart from glycerol monooleate, Table 3-13 contains also data for glycerol monoricinolate. The enzymatic process allows the production of a completely pure glycerol monoricinolate in one single step. In contrast, the conventional process requires several steps because it leads to many byproducts. For this reason, no straightforward comparison can be made (the comparison according to life cycle assessment rules would require complicated allocation procedures). We have nevertheless included glycerol monoricinolate because it is a product with outstanding product properties.

Product	Process type	Reaction	Reactor type	Catalyst type	Catalyst quantity (t/t oleyl oleate)	Reaction conditions	Downstream processing	Refining
Glycerol monooleate	Conven-tional	Transesteri-fication	Stirred tank	NaOH (or KOH)	0.005 on acid charge	- 180 °C - Atmosph. pressure	1. Decantation 2. Washing	1. Short path distillation
	Enzymatic	Transesteri-fication	Basket reactor	Immobilized lipase	0.0025	- 60 °C - Atmosph. pressure	1. Crystallization (3 steps)	1. Deodori-zation 2. Drying
Glycerol monorici-nolate	Enzymatic	Esterification	Stirred tank	Immobilized lipase	0.0015	- 60 °C - 100 mbar	1. Filtration 2. Centrifugation 3. Adsorption	1. Deodori-zation 2. Drying

Table 3-13: Process parameters for the conventional and the enzymatic production of monoglycerides (Vicente, M.; Aracil, J.; Martinez, M. 2005a; data on catalyst use originate from industry sources)

According to the economic analysis for glycerol monooleate, the simpler process scheme of the enzymatic process allows savings in capital expenditures of 5 million €, which translates to an advantage for the enzymatic process of 150 €/t glycerol monooleate for a plant with an annual capacity of 10 kt p.a. By analogy with the reasoning for oleyl oleate we conclude that the enzymatic process is economically advantageous if enzyme costs are below 150 €/ton glycerol monooleate for a 10 kt p.a. plant. For a 100 kt p.a. plant, the enzyme cost needs to be 50 €/ton glycerol monooleate or lower in order to ensure economic feasibility. Given the enzyme requirements this translates to an acceptable enzyme costs of 60 €/kg enzyme for *transesterification* in a 10 kt plant and 20 €/kg in a 100 kt plant. For *esterification*, the respective values are 100 €/kg enzyme for a 10 kt plant and 35 €/kg in a 100 kt plant. This data is shown in Figure 3-23. The comparison with the price of Lipozyme TM IM (also shown in Figure 3-23) shows that the *enzymatic* esterification in a 10 kt plant could be economically advantageous already today, while all other cases (*enzymatic* esterification in a 100 kt plant and transesterification both in a 10 kt plant or a 100 kt plant) would require lower enzyme costs.

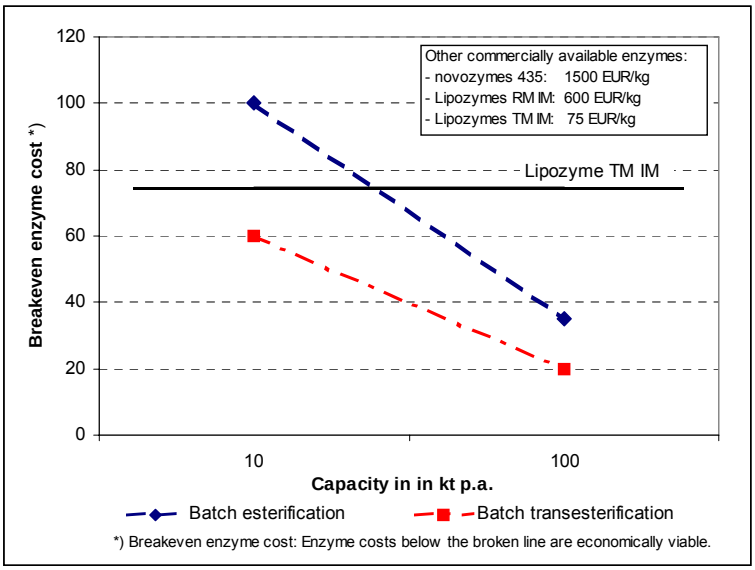

Figure 3-23: Breakeven enzyme cost for glycerol monooleate production in different reactor systems

Acrylamide

The global production of acrylamide is approximately 300,000 tonnes (Science Week 2002). Acrylamide is currently produced from acrylonitrile either by homogeneous sulfuric acid hydration or by heterogeneous catalytic hydration with a catalyst such as Raney copper. As an alternative, acrylonitrile can be converted to acrylamide by means of an enzymatic hydration process. Acrylamide is used to produce water-soluble polymers and copolymers for flocculants, papermaking aids, thickening agents, surface coatings (Ohara et al. 1997).

We compare here the conventional catalytic process using a copper oxide catalyst with an enzymatic process using Nhase Rhodococcus spec. (comparison based on data from Degussa, complemented with data from SRI (SRI-PEP91-3-3). The selectivity and yield of both processes are very high (>99%). The requirements of power, refrigeration, process water are lower for the enzymatic process and less wastewater is produced. However, the enzymatic process requires nitrogen which is not needed for the conventional process. *Direct* energy use (NREU) is estimated at approximately 8 GJ/t acrylamide for the conventional and approx. 6 GJ/t for the enzymatic process. Inclusion of the *indirect* energy use for the production of the copper oxide catalyst and the enzyme (in both cases less than 2 kg per tonne are required) results in values for total non-renewable energy use (NREU). Depending on the energy requirements assumed for enzyme production (as above assumed to lie between 15 GJ/t enzyme and 125 GJ/t enzyme, see Table 3-11) total NREU of the enzymatic process is somewhat lower (by 20%-25% or 1.6-1.8 GJ/t acrylamide).[69] The cost analysis shows lower expenses for utilities for the enzymatic process. To complete the analysis, the cost of the catalysts need to be taken into account. As a consequence of current enzyme cost (assumption: 100 €/kg enzyme), the production cost (excluding cost for acrylonitrile feedstock) are higher for the enzymatic process by around 170 €/t acrylamide but the expected

[69] Total NREU values reported here exclude the non-renewable energy use of the feedstock acrylonitrile which is identical in both processes. Inclusion of the non-renewable energy use for the production of the required acrylonitrile would reduce the difference between the processes even further.

future enzyme cost (assumption: 10 €/kg enzyme) make the enzymatic process somewhat more attractive.

The analysis presented excludes the cost of the raw material acrylonitrile because the quantities needed in the two processes are identical and the related costs therefore cancel out in the comparison. However, it is important to note that the contribution of the acrylonitrile to the total production cost is very high (around 70% of the product value) and any opportunity to lower feedstock cost could therefore be more effective than the transition to the enzymatic process.

Conclusions for enzymatic processes

The drivers for the industrial application of enzymatic conversions are i) higher product quality (specific products, e.g. chiral products and higher purity), ii) less waste (due to less undesired byproducts) and iii) the avoidance of auxiliaries that are undesired for their toxicity or for other reasons. Based on the four processes the following conclusions can be drawn:

- Many enzymatic processes offer limited to no improvement potential for non-renewable energy use (NREU) and greenhouse gas (GHG) emissions compared to conventional catalytic processes.
- Depending on the concrete case, enzymatic processes may allow to simplify the process, thus leading to lower investment costs and better operability.
- Economies of scale and advanced technology offer major (relative) improvements: Economies of scale allow to reduce the break-even cost of enzyme use by up to a factor of 3, while technological progress makes it possible to increase the allowable enzyme cost by a factor of 5.
- In order to enable economic viability on a wide scale, enzyme costs for small-scale processes (around 10 kt p.a.) would need to drop to around 100 €/kg, while enzyme costs for for larger scale processes (around 100 kt p.a.) would need to drop to a few tens of Euros per kg of enzyme; major cost reductions of this magnitude seem feasible.

To summarize, the synergy of enzymatic processes and improvements in separation processes is expected to offer new opportunities for cost reductions, while the improvement potential for non-renewable energy use (NREU) and greenhouse gas (GHG) may be very limited or even naught in many cases. At the same time, enzymatic processes allow to perform conversions and to yield specific products (e.g. enantiomers or ultrapure products) which may not be obtainable otherwise. It is also very likely that enzymatic conversions will play a key role in commercial future processes for the conversion of lignocellulosics to fermentable sugar. If process features and the economics allow to implement this type of process at large scale, it would offer major advantages in terms of non-renewable energy use and GHG emissions (see Section 3.4 and 4). In this sense, enzymatic processes are crucial for a future chemical industry applying White Biotechnology to produce bio-based bulk chemicals.

4. Scenario projections for White Biotechnology products[70]

In order to estimate the total benefits that bio-based chemicals may generate in Europe the magnitude of future production in physical terms has to be estimated. While several studies deal with the possibilities of bio-based and/or biotechnological chemical production, only very few estimates have been made about possible quantities of bio-based bulk chemicals. The estimates are either restricted to projections on the *economic* importance of White Biotechnology (EuropaBio 2003) or they exclude bulk chemicals partly or completely (Crank et al., 2005; ECCP 2001). Moreover, they are hardly ever based on a thorough analysis of process economics and of markets. As a consequence, the future market potentials of bio-based bulk chemical production are largely unknown.

Therefore, this chapter provides projections of the market potential for bulk chemicals and intermediates produced by biotechnological processes. It links back to the emerging products/processes presented in Chapter 2. A number of scenarios are distinguished to describe the possible future development of the biotechnological production of bulk chemicals in the next three to five decades. In these scenarios, different assumptions are made about the overall economic development and key inputs in the EU chemical sector. By means of scenario calculations the total requirements of land use, energy savings, greenhouse gas emission abatement and the total production value based on White Biotechnology are elaborated. We perform these scenario calculations for Europe 25 (EU-25). We limit ourselves to fermentation products and hence exclude enzymatically produced chemicals. The reasons are firstly that only very few enzymatically produced chemicals were analyzed in this study (therefore not allowing to prepare estimates at the macroscale), secondly the fact that they offer very low to no improvement potential for non-renewable energy use (NREU) and greenhouse gas (GHG) emissions (see Section 3.4.5) and thirdly, the confidentiality of costs for specific enzymes which limits the possibilities for detailed analysis. When studying fermentation products we analyze only products based on fermentable sugar from starch and from lignocelllulosice while we exclude sugar cane because it is no option for Europe.[71]

In this chapter, we review in Section 4.1 top-down market projections of bio-based chemicals. The methodology applied in our scenario analysis is described in Section 4.2. In Section 4.3, bio-based chemicals that seem most important in terms of future market volumes are selected for further investigation and their characteristics and possible petrochemical substitutions are discussed. The assumptions in the various scenarios are given in Section 4.4. In Section 4.5, market potentials of all selected bio-based chemicals are presented as well as the overall environmental and economic benefits. Section 4.6 finalizes this chapter with a discussion and conclusions.

[70] The authors of this chapter are Dr. Veronika Dornburg (main author) and Dr. Martin Patel (co-author), Utrecht University, Department of Science, Technology and Society (STS) / Copernicus Institute, Utrecht, Netherlands. Many other partners of the BREW project have contributed methodological concepts and data which were crucial for the preparation of the text in its current shape.

[71] For the economic analysis, a distinction is only made between price levels for fermentable sugar but not between feedstock types. However, for the environmental analysis, the results differ depending on whether fermentable sugar originates from starch, lignocellulosics or sugar cane.

4.1 Top-down market projections

Market projections for new products are often qualitative, because of uncertainties around market demands, market prices and diffusion processes. However, some general quantitative estimates have been made which are summarized in Table 4-1.

Most estimates for bio-based products are moderate with relatively low market shares. A larger potential is seen in the biotechnological production of chemicals of which only some are based on biomass resources (BACAS 2004; EC 2001). It should be noted that none of the market potentials presented in Table 4-1 represents exactly the product group studied in the BREW project, i.e. bio-based bulk chemicals and intermediates that are produced biotechnologically, nor the complete timeframe up to 2050. Instead, most studies deal with bio-based polymers or otherwise with bulk chemicals and in one case with solvents. Only the study of the U.S. Department of Energy (DOE) that formulates a vision—but no market potentials—for a bio-based economy comprises all bio-based bulk chemicals until 2050. The targets for bio-based chemicals put forward by this study are rather high with a 50% market in 2050, but no statement is made under which circumstances such a market potential may be realistic.

Kind of product	Market share	Year	Remarks and Reference
Biotechnologically produced building blocks	6-12%	2010	Not necessarily bio-based; ETPSC, 2004 and EuropaBio, 2003, both citing Mc Kinsey.
Bio-based polymers	1.5-3%	2010	Depending on policies; ECCP, 2001.
Bio-based solvents	12.5%	2010	ECCP, 2001.
Bio-based polymers	3-6%	2020	We assumed a total demand of 70,000 kton; Käb, 2002
Bio-based polymers	1-3%	2020	Depending on policies; Crank et al., 2005
Bio-based polymers	4%	2020	Phylipsen, et al. 2004
Bio-based chemical building blocks	10%	2020	Directional target in strategic vision; DOE, 1998
Bio-based chemical building blocks	50%	2050	Directional target in strategic vision; DOE, 1998

Table 4-1: Top-down market projections of bio-based chemicals

As shown in Figure 4-1 the future shares of bio-based bulk chemicals estimated by the partners of the BREW project vary widely. The estimates are the result of an ad-hoc poll; while they are not based on a thorough market research they reflect the various companies' expectations that are based on quantitative analyses for selected products. In Figure 4-1, two types of projections are shown, i.e. for market shares and for policy targets comparable to the strategic vision of DOE (1998).

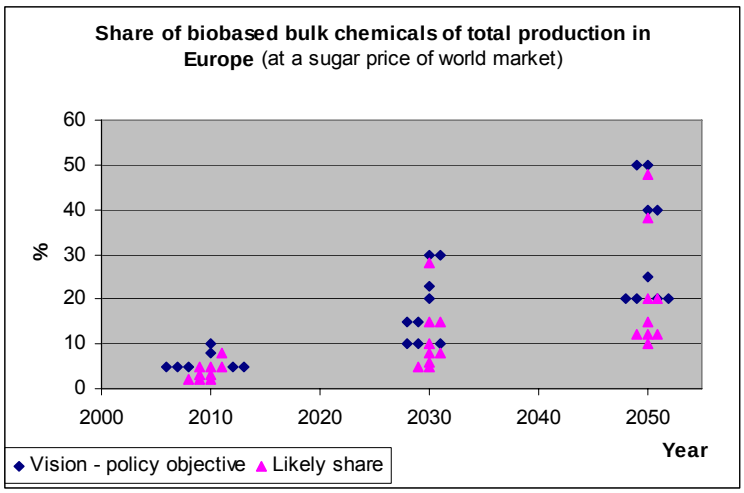

Figure 4-1: Estimates of the potential of bio-based bulk chemicals by the BREW partners

4.2 Methodology

For each scenario, the market potentials of bio-based chemicals are calculated in three different steps (see Figure 4-2). First, the technical potential of a bio-based chemical is determined, i.e. the potential to substitute a selected reference petrochemical as far as product properties allow. Second, the economic potential is determined: the economic potential is the economically viable part of the technical potential and it is a function of the difference between product values (production costs plus profit; see Section 3.3. for the methodology). Third, a diffusion rate, i.e. the time path for achieving this economic market potential is assumed, leading to the market potential for each bio-based chemical. Market potentials are calculated in steps of 10 years from 2010 to 2050.

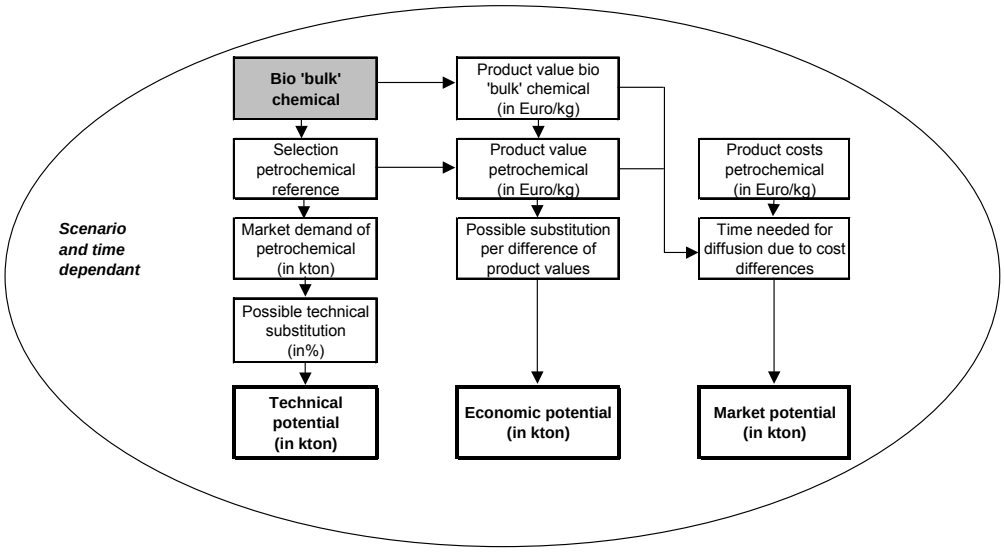

Figure 4-2: Steps to calculate the market potential of each bio-based chemical

4.2.1 Technical substitution potential

For each bio-based chemical regarded in this chapter, one or two reference petrochemicals are selected (e.g., HDPE for PHA; see Section 4.3). For the selected reference petrochemicals the future market demand in Europe is projected from the market volume in 2000 and the expected growth rate of physical production in the European chemical industry. The latter varies for the three scenarios and will be discussed in Section 4.4.

Two main types of substitution of bio-based chemicals for petrochemicals can be distinguished. Firstly, a bio-based chemical can be identical with a common petrochemical product, e.g. bio-based polytrimethylene terephthalate (PTT) could substitute fossil based PTT. In this case the technical substitution potential is 100%. Secondly, a bio-based chemical may replace a petrochemical product that is chemically different, e.g. bio-based ethyl lactate could substitute ethyl acetate. Typically, a reference petrochemical is used for a broad variety of applications for which the bio-based alternative is more or less suitable. Therefore, it is difficult to determine, in quantitative terms, the technical substitution potential exactly for each application and to aggregate these values to a total substitution potential. Instead we use overall estimates of the BREW partners on the suitability of bio-based chemicals for the substitution of reference petrochemicals (see Section 4.3 for the resulting substitution rates).

4.2.2 Economic substitution potential

For the calculation of economic substitution potential, two cases are distinguished, too. First, if the same chemical is substituted, the economic substitution potential is 100% in case the product value of the bio-based chemical is lower than the product value of the petrochemical. Otherwise, the economic substitution potential is 0%.

Second, if a different chemical is substituted, the economic substitution potential depends on the ratio between the product value of the bio-based chemical and the product value of the petrochemical (see Figure 4-3). However, the substitution rates, had to be estimated in rough way as no methodology to quantify such substitution rates could be identified in literature. Furthermore, important parameters, as the willingness to pay for certain product advantages and the application mix of petrochemical products are unknown, too.

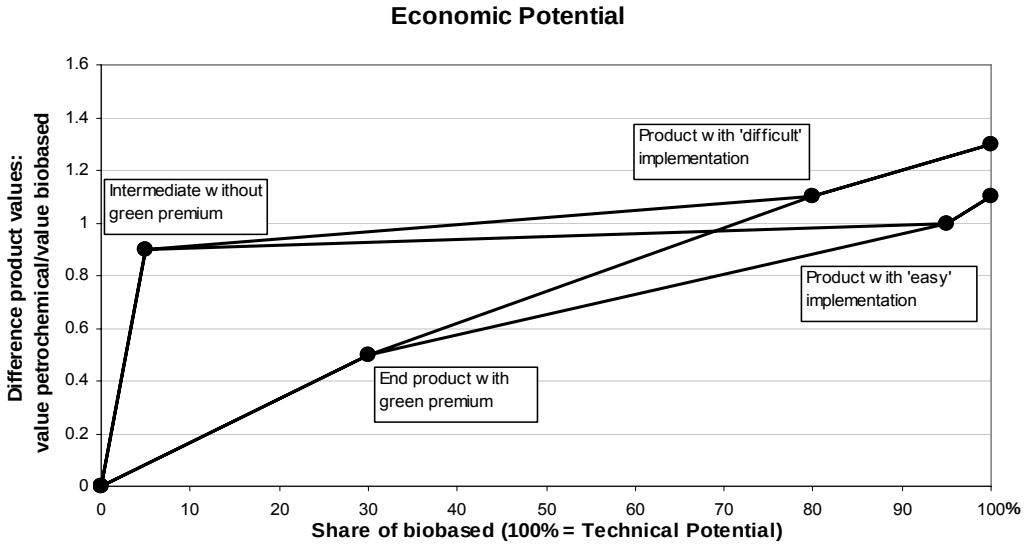

Figure 4-3: Economic market potentials depending on the difference of product values of a bio-based chemical and a reference petrochemical

Economic substitution rates applied in this study are estimated from general product characteristics (see also Section 4.3.2). First, it is estimated whether a chemical is eligible to a "green premium". This means that a bio-based chemical has ecological or functional advantages that lead to substantial substitution even if its product value (i.e., the profited production cost) is larger than for its petrochemical equivalent. In this study, it is assumed that only end products (such as polymers) have such a "green premium", while intermediates (e.g. acetic acid) have not. Second, it is estimated whether a bio-based chemical is easy to implement or not. Bio-based products that are difficult to implement have disadvantages compared to their petrochemical counterparts and therefore do not substitute these completely until the product value is much lower. It is assumed that bio-based chemicals with rather different product properties than their petrochemical counterpart are difficult to implement.

4.2.3 Technology diffusion

The time required for the diffusion of bio-based chemicals depends on the level of their product values in comparison with the product values of petrochemical counterparts. In consultation with the chemical industry experts in BREW, it has been assumed that it takes 30 years until the full economic potential is reached,[72] if the product value of the bio-based chemical is not lower than the depreciated production costs (i.e., the production costs without depreciation) of the reference petrochemical. This implies that existing depreciated petrochemical production facilities are kept in place until their end of life. If the product value of the bio-based chemical is lower than the depreciated production costs of the reference petrochemical, the time to reach the full economic potential is assumed to be 10 years. This means that existing petrochemical production facility is shut down before its technical end of life. However, if the demand for chemicals grows fast and additional capacity is anyway

[72] Over 30 years, thus, the diffusion potential rises linearly until the full economic potential is reached.

needed (this implies that bio-based chemicals do not have to compete with depreciated plants), the diffusion time for this capacity is assumed to be zero. Thus, the economic potential of bio-based chemicals is assumed to materialize immediately in order to satisfy the growing demand.

4.3 Bio-based chemicals and reference petrochemicals

4.3.1 Selection of products

Many intermediates and derivatives can be produced from biomass. An overview of the possibilities for substitution has been given in Chapter 2 of this report. For the analysis of market potentials, the bio-based intermediates and derivatives shown in Table 4-2 have been selected. These products were selected because the BREW team considered these products to be potential candidates for large-scale use. The main criterion for this selection was the outcome of the economic analysis presented in Chapter 3 (Table 3-10) in combination with the assessment by the BREW team according to which these bio-based products may be good candidates for gaining large market shares (in physical terms). This implies, that the (future) production costs of these bio-based chemicals are expected to be comparatively low, while the total market demand is relatively high. Making this selection, we limit the data requirements for the analysis to a reasonable level, but as a consequence, a couple of products that have been included in the economic and environmental analysis in Chapter 3 are not further considered. These are acrylic acid, caprolactam, ethanol[73] and lysine. These products have been excluded because they have a relatively small market potential as bulk chemicals and because a thorough analysis would need to take into account intersubstitution with the other chemicals studied, e.g. the fact that the competition between petrochemical nylon 6 and bio-based PTT (see Table 4-2) would be further complicated by the existence of bio-based nylon 6 (derived from bio-based caprolactam). Apart from the exclusion of these products also all chemicals produced by enzymatic processes have been excluded, as explained at the beginning of Chapter 4.

For each of the selected bio-based chemicals, petrochemicals have been identified that are most likely to be substituted (Table 4-2). This list of reference petrochemicals was chosen by the members of the BREW team. It hence includes implicit expectation on markets, e.g. polymer markets, and technical properties of the chemicals in question. In most cases, one main reference petrochemical has been identified, while in some cases two different reference petrochemicals are considered.

[73] (Bio-)Ethylene from bio-based ethanol is, however, included.

Bio-based chemical	Reference petrochemical 1	Reference petrochemical 2
PHA	HDPE	-
PTT	PTT [1)]	Nylon 6 [1)]
PLA	PET [2)]	PS [2)]
Ethyl lactate	Ethyl acetate	-
Ethylene	Ethylene	-
Succinic Acid	Maleic Anhydride	-
Adipic acid	Adipic acid	-
Acetic acid	Acetic acid	-
n-Butanol	n-Butanol	-

1) Contrary to the choice made here, petrochemical polyethylene terephthalate (PET) has been chosen as reference in Chapter 3. The reason is that scenario-dependent economic analyses (as discussed in this Chapter 4) are required in order to establish the bio-based shares of the PTT market (reference petrochemical 1) and of the nylon 6 market (reference petrochemical 2). The cradle-to-factory gate NREU of petrochemical PTT (73.5 GJ/t) and of petrochemical nylon 6 (119.5 GJ/t) embraces the value for petrochemical PET (77.2 GJ/t; amorphous PET).

2) Contrary to the choice made here, petrochemical polyethylene terephthalate (PET) has been chosen as reference in Chapter 3. The reason analogous to the one given in footnote 1). The cradle-to-factory gate NREU of petrochemical PET (77.2 GJ/t); amorphous PET is smaller than that of petrochemical PS (86.7 GJ/t; value for General Purpose Polystyrene, GPPS).

Data on cradle-to-factory gate NREU were taken from Boustead et al. (various years).

Table 4-2: Selected bio-based chemicals and petrochemical counterparts

Acetic acid, adipic acid ethylene and *n*-butanol are intermediates that are already produced in relatively high volumes from fossil resources. Chemically identical compounds made from biofeedstocks could replace these compounds. In contrast, the polymers shown in Table 4-2 (i.e. PHA, PLA, PTT) are not produced petrochemically in large quantitites. Consequently, it is assumed that they replace other petrochemical bulk polymers such as nylon 6, PE, PS and PET. Moreover, bio-based PTT also substitutes for fossil based PTT, which is currently produced in rather small quantities. As polyethylene is produced from ethylene, in our scenarios either the polyethylene can be replaced by the bio-based polymer PHA or the ethylene needed can be produced from bio-based ethanol.

Ethyl lactate and succinic acid are further examples of products that are not produced in large quantities from fossil resources. Therefore, bio-based ethyl lactate and bio-based succinic acid have a limited market for *direct* substitution but they do have the potential to replace other petrochemicals. Ethyl lactate is an organic solvent that can, among others, substitute ethyl acetate on a large scale. Succinic acid can be an intermediate for the production of 1,4-butanediol, tetrahydrofuran and polyesters. It is compared to maleic anhydride, which is mainly used for the production of 1,4-butanediol, polyesters and tetrahydrofuran.

4.3.2 Input data

In this section, the input data assumed for our market projections are described. As discussed in Section 3.1, several process flow diagrams were developed and evaluated for each chemical (the process schemes differ with regard to the biotechnological step and the product workup; see Appendix A9 for all diagrams). Out of these diagrams, we chose, for each product, the economically most attractive process options for projecting the future market potential. However, the point of time at which the transition is made from state of the art processes to future processes differs depending on the scenario (see below, Section 4.4). The process data used refer to a capacity of 100 kton/yr for the bio-based chemicals. For the production of

petrochemicals, a typical world scale process has been assumed (i.e. the largest scales stated in SRI, 2000; see Table A10-1b).

The *technical substitution potentials* for the substitution of petrochemicals by bio-based chemicals have been estimated roughly by the experts in the BREW team; the data are shown in Table 4-3. For those cases where the bio-based and the petrochemical product are chemically identical the technical substitution potential is 100% (not shown in Table 4-3).

Bio-based chemical	Petrochemical	Technical substitution potential (in %)
PHA	PE	25
PTT	Nylon 6	100
PLA	PET	90
PLA	PS	100
Ethyl lactate	Ethyl acetate	100
Succinic Acid	Maleic Anhydride	85

Table 4-3: Technical substitution potential (for years 2010 to 2050) of the bio-based chemicals and their petrochemical counterparts studied

Finally, the eligibility of bio-based chemicals for a "green premium" (only for end products) has been specified and their implementability has been estimated (Table 4-4). These parameters determine the *economic potential* of bio-based polymers. A quantification of these assumptions can be found in the appendix in Table A12-2.

Bio-based chemical	Reference petrochemical	Green premium	Implementation
PHA	HDPE	Green premium	Difficult
PTT	Nylon 6	Green premium	Easy
PLA	PET	Green premium	Difficult
PLA	PS	Green premium	Difficult
Ethyl lactate	Ethyl acetate	Without	Difficult
Succinic Acid	Maleic Anhydride	Without	Difficult

Tabe 4-4: Eligibility for green premium and implementability for bio-based chemicals replacing non-identical petrochemicals

4.4 Scenario assumptions

Market potentials of bio-based chemicals depend on many factors such as fossil fuel prices, other raw material prices, process technology development etc. As these factors could evolve very differently in the next 5 decades, the market conditions for bio-based chemicals could differ substantially. We therefore investigate market potentials for various scenarios. The projections of market potentials are hence not to be seen as forecasts but rather as expectations under pre-set conditions; given the time required for the full development of most processes followed by gradual diffusion and replacement of the existing capital stock, a time period of 50 years seems appropriate.

Many potential images of the future exist. In order to explore the range of possible market potentials, we restrict the analysis to three rather simple scenarios:

- LOW: In this scenario, external factors are disadvantageous for the development and implementation of bio-based chemicals. The expected market potentials are therefore low.
- MEDIUM: Conditions for the utilization of bio-based chemicals are neither especially advantageous nor disadvantageous. As a consequence, market potentials are anticipated to be medium.
- HIGH: Finally, in this scenario all assumptions favor the market potentials of bio-based chemicals, which in turn are estimated to be high.

Out of the large number of parameters that influence the market potentials of bio-based chemicals (compare Crank et al. 2005) we limit ourselves in this study to the factors that the experts within the BREW team have identified to be the most important. Table 4-5 gives an overview of the main assumptions concerning these factors in the three scenarios.

Scenario	LOW	MEDIUM	HIGH
	Bad conditions for bio-based chemicals	Medium conditions for bio-based chemicals	Good conditions for bio-based chemicals –
Fossil fuel prices	Low (up to 30 US$/barrel)	Medium (up to 66 US$/barrel)	High (up to 83 US$/barrel)
Technological development	Low, technology remains at current state of the art (economically best options are chosen)	Future technologies are available from 2040 onwards (economically best options are chosen)	Future technologies are available from 2020 onwards (economically best options arechosen)
Bio-feedstock costs	High (400 €/t fermentable sugar)	Medium (200 €/t fermentable sugar)	Low (70 €/t fermentable sugar)
Market chemicals	No growth (0% p.a.)	Medium growth (1.5% p.a.)	High growth (3% p.a.)
Subsidies	No subsidies for bio-based chemicals	No subsidies for bio-based chemicals	Subsidies for bio-based chemicals (1 to 5% of product value)

Table 4-5: Main assumptions in the three different scenarios

4.4.1 Fossil fuel prices

Projections of future fossil fuel prices vary largely with respect to time frames as well as price levels. For example, the U.S. Department of Energy estimates crude oil prices to be in the range of 40 to 65 US$/barrel in 2005 to mid 2006 (DOE 2005), while in 2005 the investment bank Goldman, Sachs projected very high peak prices of 105 US$/barrel in the short term (Independent 2005). The World Energy Outlook (IEA 2004) estimates that in the next couple of years after 2004 crude oil prices will drop below 30 US$/barrel. The “high oil price scenario” of the World Energy Outlook assumes a price of 35 US$/barrel until 2030 (IEA 2004). Similarly, Lako and de Vries (1999) have published moderate estimates: For the year 2020 crude oil prices are projected to be in the range of 15-30 $US\$_{98}$/barrel and for the year 2050 in the range of 20-35 $US\$_{98}$/barrel.

The IPCC developed a couple of scenarios to estimate future GHG emissions that are based on different economic and political developments (IPCC SRES 2000). The resulting GHG emissions are calculated with several models. Some of these models also calculate fossil fuel price developments for the different scenarios (an overview of different model results on fuel

prices for the SRES scenarios is given in the Appendix, Table A11-1). One of the models which was used for the SRES report and which contains fossil fuel prices projections is the Message model. In this study, we used the fossil fuel prices from the Message model for our market projections for the coming 5 decades. Fuel prices in our LOW scenario are represented by the B1 scenario, in our MEDIUM scenario by the B2 scenario and in our HIGH scenario by the A2 scenario. In order to make our scenarios consistent - i.e., to ensure that in each year the fossil fuel price is highest in the HIGH scenario - we linearised the fossil fuel price trends (see Figure 4-4). It should hence be noted that fossil fuel prices in our scenarios are no projections of future crude oil price, but represent different images of the future under certain circumstances. Using **a value of 25 US$/barrel as a price base**, crude oil prices in our scenarios range from **30 to 66 and 83 US$/barrel in 2050** in the three scenarios.

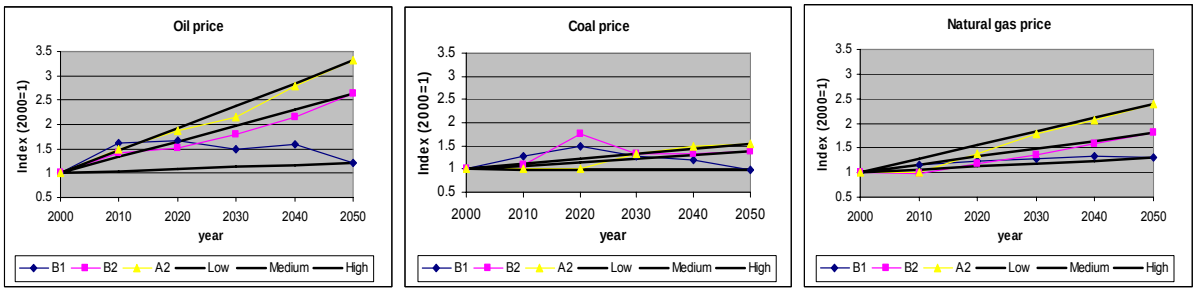

Figure 4-4: Fossil fuel prices in the three different scenarios

Fossil fuel prices influence the production costs of bulk chemicals in two ways. First, fossil fuels are direct inputs in the production process and as such influence the production costs. Second, fossil fuels are inputs for the production of utilities and intermediate chemicals, which are used for the production of the considered bulk chemicals. We estimated the prices of these utilities and intermediates as a function of fossil fuel prices: For steam production average data of the European chemical industry were used as starting point (see Apendix A3.2). As steam production requires only a modest amount of investment, we assumed that about 95% of the steam price is related to natural gas prices. Refrigeration and compressed air are also assumed to depend for 95% on energy costs, i.e. on electricity prices. For inert gas, cooling water and process water, we use identical prices in all three scenarios. Prices of other fuels than crude oil, coal and natural gas assumed to increase proportionally to natural gas or crude oil prices. Naphtha prices have been assumed to develop proportionally to crude oil prices. This relation has been determined from fitting of historical data (see Appendix A11-4). Concerning electricity, prices in the various scenarios are calculated based on the current average shares of energy carriers in European electricity production and techno-economic data on power generation; see Appendix A11-2.

The future product value of very important intermediates for the production of bio-based chemicals (i.e., bio-ethanol and bio-PDO) has been calculated by using the methodology explained in Section 3.3. The methodology has also been used to calculate the future product values of the petrochemical intermediates propylene, ethanol, terephthalic acid, dimethyl terephthalate, ethylene glycol, ethylene oxide, acetylene, p-xylene, caprolactam and styrene. For other intermediates and raw materials (e.g., acetaldehyde, benzene and xylenes), which are used in rather small quantities for the production of bio-based products, prices were taken from SRI reports and were adjusted to changed fossil fuel and utility prices. This has been done using the shares of these inputs to the total production costs. If no process data are

available, the prices of feedstock were adjusted to the price changes of their main petrochemical feedstock (natural gas or oil products; see Appendix A11-3). For auxiliaries and catalysts, often no detailed data of the cost structure were available. As approximation, it has been assumed that 30% of the prices of auxiliaries change with crude oil prices. The prices of catalysts, that mainly comprise metal compounds and enzymes, are not assumed to change as a function of fossil fuel prices because, for these products, (direct) energy costs generally represent a very small part of the final product price.

4.4.2 Technological developments in White Biotechnology

In BREWtool different datasets for the production of biotechnologically produced chemicals have been developed (see Chapter 3). These datasets describe state of the art technologies (TODAY; see Chapter 3) as well as FUTURE technologies. In the LOW scenario, no significant technological development is assumed to take place. As a consequence, today's state of the art technologies for the production of bio-based chemicals are assumed to be used until the year 2050. On the other hand, technological development proceeds at a fast pace in the HIGH scenario. In this scenario, we assume future technologies for the production of bio-based chemicals to become available from 2020 onwards. Since the intensity of R&D influences the timeframe for the development of new technologies, it is assumed that in the MEDIUM scenario technology development is slower. Here, future technologies are available from 2040 onwards only. Both for state of the art technologies and for future technologies we always choose the economically best option (lowest production cost) for our scenario projections.

4.4.3 Bio-feedstock costs and land availability

Chemicals produced by fermentation can be derived from fermentable sugar, from vegetable oils, glycerol and other feedstocks. Wherever data were available, the production from feedstocks other than fermentable sugar was analyzed in Chapter 3. Since our calculation results for these other feedstocks were less advantageous we limit ourselves in the scenario projections to fermentable sugar as feedstock for the bio-based chemicals. This fermentable sugar can be derived from many sources, e.g. via starch from corn or wheat or via lignocelluloses from stover, straw or short rotation wood (see Chapter 3). In the economic analyses performed as part of the scenario projections presented in this chapter, the source of fermentable sugar remains, however, undefined. Instead, different price levels for fermentable sugar are assumed. As for fossil fuel price, these prices may vary widely. Current prices of fermentable sugar from sugar cane vary between 70 and 240 US$/ton (see Appendix A6), while prices of fermentable sugar in Europe are around 300 €/ton.[74] Prices of fermentable sugar from lignocellulosics could be in the range of about 30 to 160 €/ton. The price levels for fermentable sugar assumed in BREWtool are 70, 135 and 200 and 400 €/t (see Section 3.4.1). These price levels are also used for the scenario analysis. In the HIGH scenario, a low sugar price of 70 €/t is assumed, which approximately represents current sugar prices in Brazil and is the lowest price level currently achieved worldwide. Thus, this scenario represents a "free"

[74] This represents the current price of sugar made from starch crops in Europe. Sugar production from sugar beet in Europe is decisively more expensive, costing around 700 €/t but the higher production cost is currently compensated by subsidies for industrial use of sugar (about 400 €/t). These subsidies for sugar production from sugar beet will be gradually removed over the next few years. As a consequence, sugar industry in Europe will be restructured, shifting from sugar beet to starch as raw material.

sugar market without trade limitations and without limitation of agricultural land availability or, alternatively, the location of the fermentation plant in a tropical country producing sugar cane. In the MEDIUM scenario, a sugar price of 200 €/t is assumed. This is about the current price of sugar in the US (see Table A5-2). It is lower than the current sugar prices in Europe (approx. 300 €/t) due to better production conditions and ample availability of land in the U.S. Finally, in the LOW scenario a very high sugar price of 400 €/t is assumed. This is beyond the current average sugar price in Europe and could be reached as a consequence of competition for agricultural land with the production of bio-energy and food and/or an agricultural policy that prevents the decrease of sugar prices.

We assume the prices of by-products of corn starch production (e.g., of corn steep liquor) to change with the same ratio as sugar prices. However, these nutrients only have a minor share of total costs of bio-feedstocks and therefore hardly influence the price of the final product.

4.4.4 Chemical market

The demand for petrochemicals is projected using annual growth rates. The starting point for these projections is the current production volume of chemicals in 2000 in the EU-25. As shown in Table 4-6 production data are only available for Western Europe for many chemicals. However, the production in the Accession States of Central Eastern Europe is low in most cases (compare Table 4-6). Using a variety of sources we estimated the *total production of all organic chemicals* in EU-25 in the year 2000 at approximately **70 million tonnes**.[75]

Future developments in the chemical industry are uncertain. On the one hand, the production of chemicals in Europe depends on the global chemical demand, which in turn is influenced by the overall economic development. On the other hand, the production in Europe is also influenced by the competitive position the European chemical industry achieves. Based on discussions within the BREW team, a low growth rate of 0%, a high growth rate of 3% p.a. and a medium growth rate of 1.5% p.a. were assumed (see Table 4-5). These projections are within the range of projection from other scenario analyses (see Appendix A11-5). As a consequence, the ***total production of all organic chemicals*** in 2050 is projected to amount to 70 million tonnes in the LOW scenario (same value as in year 2000), 150 million tonnes in the MEDIUM scenario **and 300 Mt in the HIGH scenario**.

The total *production of the selected chemicals* (i.e. promising bulk chemicals that can be replaced by White Biotechnology products from bio-based resources; see Table 4-2) in EU-25 was about 31 million tonnes in the year 2000 (Table 4-6). When calculating this total we avoided double counting of ethylene as such and in the form of polyethylene (instead only ethylene was taken into account in the total while polyethylene was omitted) and the inputs of ethylene for other products given in Table 4-6. Apart from this case the production of acetic acid *may* involve the use of ethylene and the manufacture of ethylacetate, polyethylene

[75] Based on the insight gained from detailed material flow analyses of the petrochemical sector in the Netherlands and in Germany (Neelis et al., forthcoming a and b; Weiss et al. 2005) it has been estimated that the total production of all organic chemicals (without double counting related to intermediates) can be estimated by multiplying the total production of polymers by a factor of 1.35. For Germany and the Netherlands, the resulting values represent 92-99% of the chemical feedstock use reported in international energy balances (IEA 2003). This is a plausible result considering that on the one hand part of the feedstock is oxidised and that on the other hand heteroatoms (esp. nitrogen and oxygen) are embodied in the final product.

terephthalate (PET) and polystyrene (PS) certainly *does* involve ethylene.[76] We have not corrected for these quantities because they represent relatively small quantities, leading to limited double counting. This is justified because there are further options for substitution which have not been taken into account such as the partial replacement of petrochemical propylene and its derivatives by bio-based ethylene and other White Biotechnology products. The total of the selected chemicals calculated in this way (31 million tonnes) represents nearly 50% of the total production of all organic chemicals in EU-25 in the year 2000 (approx. 70 million tonnes). Hence, for the year 2050, the ***total production of the selected chemicals*** **is projected to amount to 31, 65 and 136 million tonnes in the LOW, MEDIUM and HIGH scenario** (these values have also been calculated using growth rates for of 0%, 1.5% and 3% p.a. for the three scenarios; for comparison, see growth rates from other studies in Appendix A11, Table A11-5b).

Petrochemical	Volume (in kton)	Year and region	Reference
PE (HDPE, LDPE, LLDE)	11,300	2000, Western Europe[a]	CEFIC 2005a
Ethylene	19,403	2000, Western Europe	CEFIC 2005a
PTT	524	2000[b]	APME 2003
Nylon 6	1,255	2000, Western Europe[c]	APME 2003
PET	3,500	2000, EU-25[d]	APME 2003
PS	3,365	2000, EU-25[d]	APME 2003
Ethyl acetate	310	1999, Western Europe[e]	Weissermel and Arpe 2003
Maleic Anhydride	380	1999, Western Europe[f]	Weissermel and Arpe 2003
Adipic acid	1,000	1999, Western Europe[g]	Weissermel and Arpe 2003
Acetic acid	1,400	1999, Western Europe[h]	Weissermel and Arpe 2003
n-Butanol	930	1999, Western Europe[i]	Weissermel and Arpe 2003

[a] About 11700 kton ethylene are needed for the production of 11300 kton polyethylene. This demand of ethylene can only be replaced once within the market potentials.
[b] Consumption figure of other polymers in Western Europe.
[c] 44% of polyamide consumption as consumption (PA 6/66/other) for Western Europe was in the ratio of 44/46/10 in 1988. (Ullmann 1997)
[d] Consumption data. Data for PS includes expanded polystyrol.
[e] Production outside Western Europe, USA and Japan was about 510 kton in 1999.
[f] Production outside Western Europe, USA and Japan was about 530 kton in 1999.
[g] Production outside Western Europe, USA and Japan was about 390 kton in 1999.
[h] Production outside Western Europe, USA and Japan was about 3610 kton in 1999.
[i] Production volume includes all types of Butanol. Production outside Western Europe, USA and Japan was about 246 kton in 1999.

Table 4-6: Production volume of *selected chemicals* in Europe used as base chemical market demand in 2000

[76] We assumed the following petrochemical routes by making use of information from SRI reports (var. years), Ullmann (1997) and Patel et al. (1999, appendix No. 3):

- Acetic acid: made by methanol carbonylation (preferred technology esp. for future); other options are the liquid-phase oxidation of n-butane, naphtha or acetaldehyde; acetaldehyde is made from *ethylene*).
- Ethylacetate (1 t): made from acetic acid (0.68 t) and ethanol (0.52 t). Petrochemical ethanol (1 t) is made from *ethylene* (0.63 t). For acetic acid, see above.
- PE: made from *ethylene*
- PET (1 t): made from xylene (0.66 t), methanol (0.09 t) and *ethylene* (0.22 t) (via dimethylterephthalate and ethylene glycol)
- PS (1 t): made from benzene (0.85 t) and *ethylene* (0.30 t)

4.4.5 Subsidies

The production of bio-based chemicals might be stimulated by policy. To include possible policy stimulation, direct subsidies are included in the HIGH scenario. However, the level of subsidies assumed is very low: Between 2000 and 2050 a decreasing value of 5% to 1% of the product value is granted as a subsidy. Thus, the market potentials in the HIGH scenario are hardly influenced by these subsidies (see below).

4.5 Market projections

4.5.1 Market potentials

The market potentials for the three scenarios are depicted in Figure 4-5. The lower part shows the bio-based products, produced by White Biotechnology. These increasingly substitute a share of the *selected organic chemicals* (listed in Table 4-6). The *selected organic chemicals* are approximately half of *all organic chemicals* which are represented by the upper, broken line in Figure 4-5. The total volumes differ significantly across the scenarios. While in the LOW scenario in 2050 only about 5 million tonnes of bio-based chemicals are produced, the respective values for the MEDIUM and the HIGH scenario are about 26 million tonnes and 113 million tonnes. In the HIGH scenario, the total demand for bio-based chemicals is hence about 20 times higher than in the LOW scenario. Part of this large difference can be explained by the difference in the total market demand for chemicals. Another part of this difference is due to the advanced technology and the differing raw material prices, that result in a better economic performance of bio-based chemicals than petrochemicals in the MEDIUM and HIGH scenario (see shares of bio-based chemicals below). The findings per scenario are as follows:

- In the LOW scenario, PLA has the largest market potential and also PTT and PHA have relatively large potentials. The product values of PLA and PHA are higher than those of their petrochemical counterpart, i.e. these products enter the market only on behalf of the "green premium" (see Section 4.2.2). In contrast, PTT is competitive compared to PS and it is at the edge to competitiveness compared to petrochemical PTT. Minor quantities of ethyl lactate and of succinic acid enter the market as a consequence of the "green premium".
- In the MEDIUM scenario, the most important potentials are those of PLA, PHA and PTT (as in the low scenario). Throughout the period studied PLA and PTT are economically slightly more viable than some of their petrochemical counterparts (petrochemical PET for PLA and petrochemical PTT for bio-based PTT). PHA becomes economically viable only between 2040 and 2050 but enters the market in noticeable quantities already in 2010 due to the "green premium". In the very last decade (2040-2050) also bio-based ethylene becomes economically viable and is produced.
- In the HIGH scenario, several other White Biotechnology products enter the market in addition to PLA, PTT and PHA. Most importantly, ethylene is produced in very substantial quantities from 2030 onwards. At the end of the period also adipic acid, n-Butanol, succinic acid and ethyl lactate (ordered by decreasing quantities) contribute to the overall potential but the quantities are relatively low. The product values of all bio-based products are lower than those of at least one of their petrochemical counterparts

from 2020 onwards (for ethylene from 2020 onwards). This means that the "green premium" does not contribute significantly to the market development in the second half of the HIGH scenario.

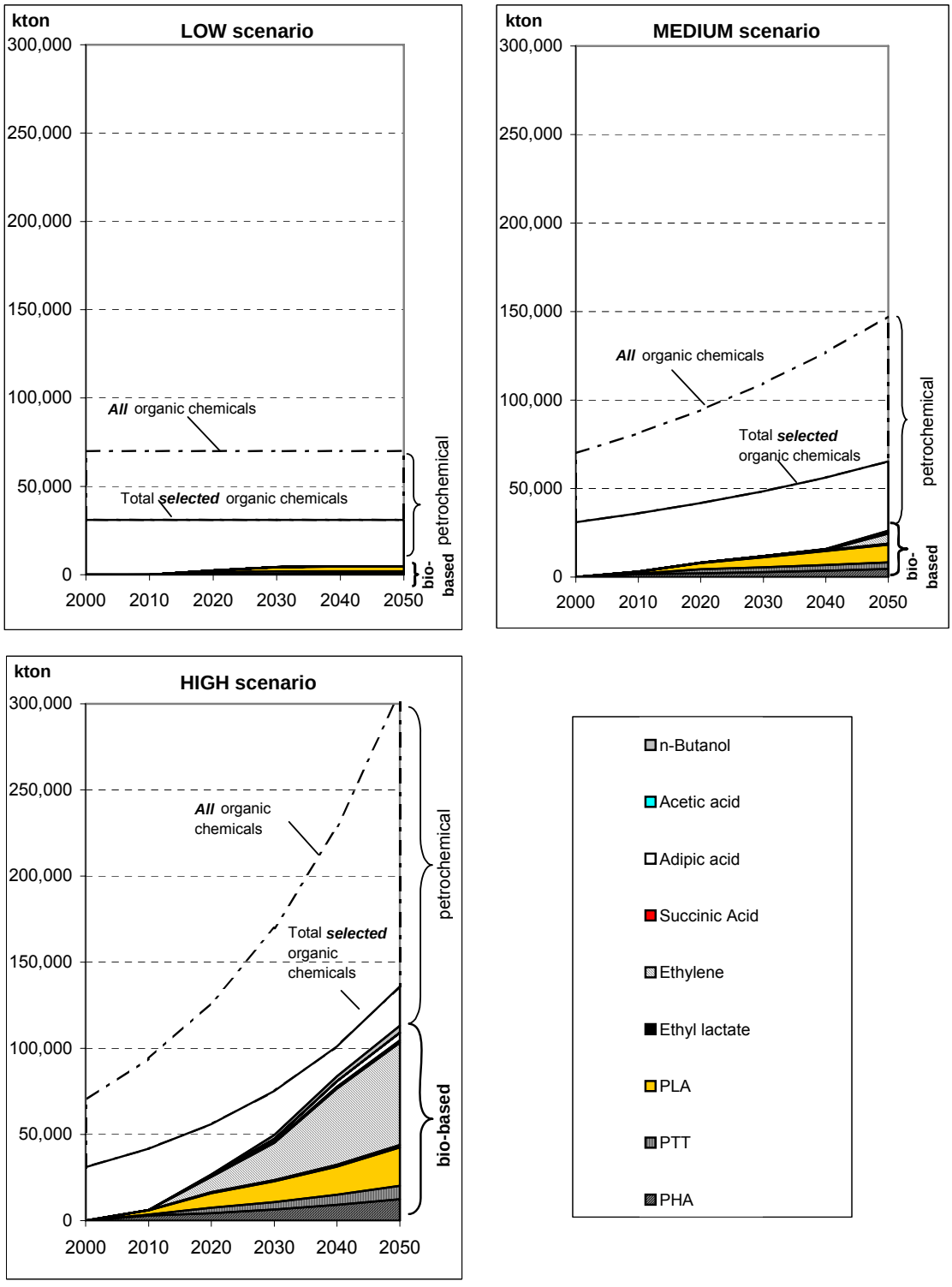

Figure 4-5: Market potentials of bio-based bulk chemicals in Europe for the three scenarios for the years 2010 to 2050

The relative shares of bio-based chemical production in relation to the total chemical demand are presented in Figure 4-6. The percentages represent the shares of the production of bio-based chemicals relative to the production of the selected petrochemical product that serves as reference (compare Table 4-2). Again, the differences between the scenarios are quite significant. The total shares of bio-based chemicals range from 15% in the LOW scenario to 40% in the MEDIUM scenario and 83% in the HIGH scenario.

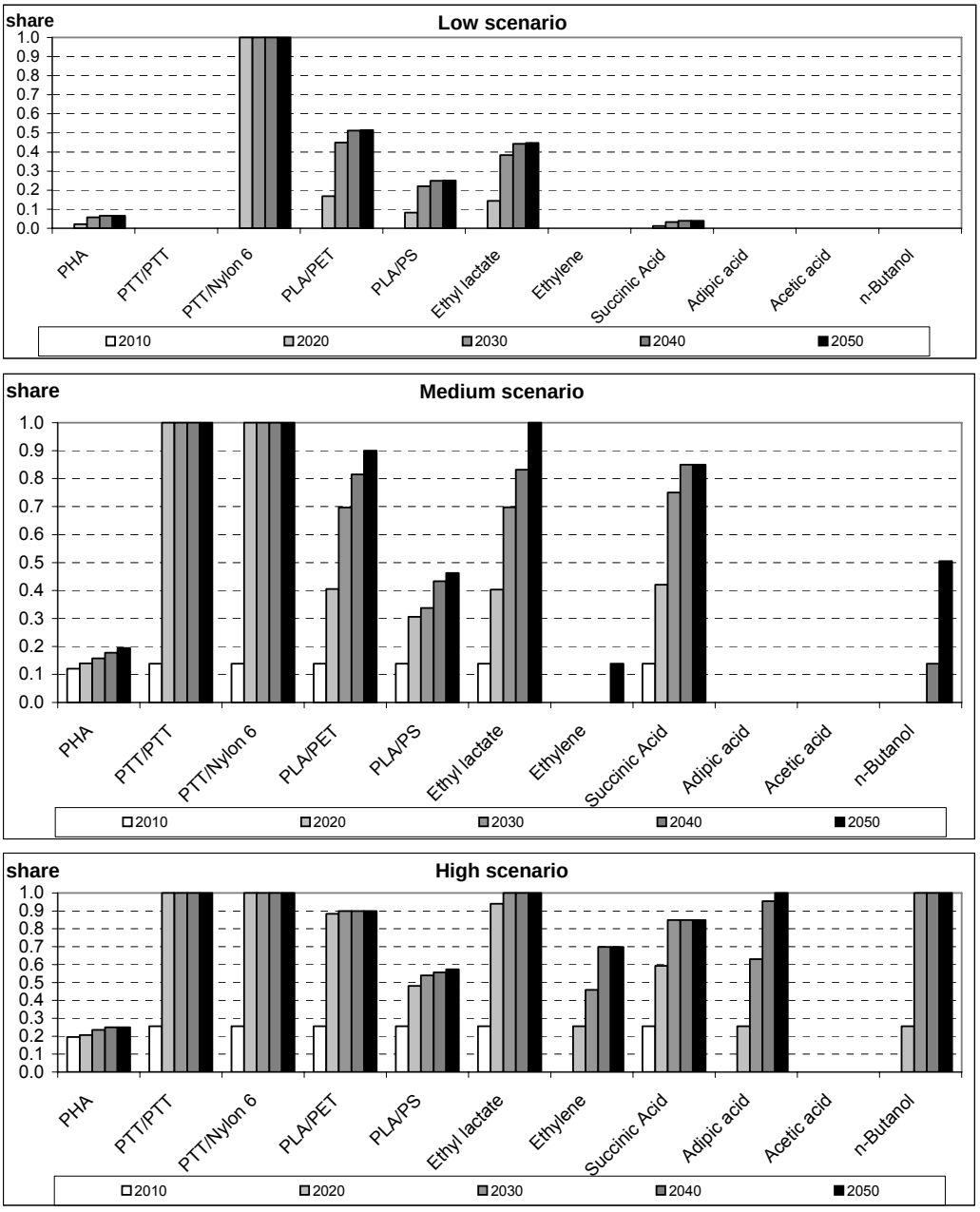

Figure 4-6: Share of bio-based chemical production relative to the selected reference petrochemical product in Europe for the three scenarios for the years 2010 to 2050

The difference between the product value of a bio-based chemical and its petrochemical counterpart range from about –3600 €/t[77] to 2500 €/t (a complete overview for all chemicals is given in Appendix A13). For some bio-based chemicals, this difference is highly dependent on technology developments, namely for succinic acid, adipic acid, acetic acid and n-butanol. For other bio-based chemicals, this difference is also strongly influenced by the scenario considered, namely for PHA and ethylene. Finally, several bio-based chemicals show a rather robust difference in product values, i.e. PTT, PLA and ethyl lactate.

As explained in Section 4.2.3 the market projections account for the time needed for diffusion of bio-based chemical production capacity. We find that the time delay for the adaptation of bio-based chemical production is significant. In Table 4-7, the market potentials (which include the delay for diffusion) and the economic potentials (which do not account for the delay) are compared. In the first decases, the economic potentials are only realized to a limited extent. In the last decade, the market potentials are in general rather close to the economic potentials (mostly between 90%-100%, with the MEDIUM scenario being an exception: bio-based ethylene becomes ecomically viable but only a small part of the potential is implemented[78]).

Potential	LOW scenario					MEDIUM scenario					HIGH scenario				
	2010	2020	2030	2040	2050	2010	2020	2030	2040	2050	2010	2020	2030	2040	2050
Market potential (kt)	0	2,415	4,352	4,779	4,794	3,083	8,208	11,930	15,977	26,249	6,190	26,731	49,727	83,848	113,117
Economic potential (kt)	4,734	4,749	4,764	4,779	4,794	8,059	9,931	12,141	18,129	57,632	11,944	51,593	69,463	93,526	125,935
Share	0.00	0.51	0.91	1.00	1.00	0.38	0.83	0.98	0.88	0.46	0.52	0.52	0.72	0.90	0.90

Table 4-7: Comparison of the market potentials (including diffusion) and the economic potentials (excluding diffusion) for bio-based chemicals

4.5.2 Economic and environmental benefits

By deducting the total of all product values of bio-based chemicals (according to the market potential) from the total of all product values of their reference petrochemicals, the achievable savings for the economy can be estimated. We refer to these savings as macroeconomic savings. The outcome for Europe is shown in Figure 4-7 and Figure 4-8. As discussed in Section 4.2.2 some bio-based chemicals have a “green premium” effect, which means that they are produced already even if product values are higher than those of the reference petrochemicals. As a consequence, the total difference of product values can be negative. This is the case in the LOW scenario between 2030 and 2050 and in the first decade for the MEDIUM scenario. However, in the second decade the total difference between product values becomes positive in the MEDIUM scenario and it is positive throughout the HIGH scenario. In 2050 the total product value savings are -0.13, 6.7 and 74.8 billion € in the three

[77] The negative difference of values indicates that the bio-based chemical has higher product value than its petrochemical counterpart. In this case the bio-based chemical is not competitive.

[78] According to our model assumptions the diffusion of ethylene production takes about 30 years because the product value of the bio-based chemical is not lower than the depreciated production costs (see Section 4.2.3).

scenarios (the negative value of -0.13 billion € for the LOW scenario represents a net loss, while the values for the scenarios MEDIUM and HIGH represent net savings). White Biotechnology hence offers substantial macroeconomic savings in the scenario HIGH and moderate savings in the scenario MEDIUM; it entails small additional expenses in the scenario LOW. The macroeconomic savings can be interpreted as an indicator for improved competitiveness.

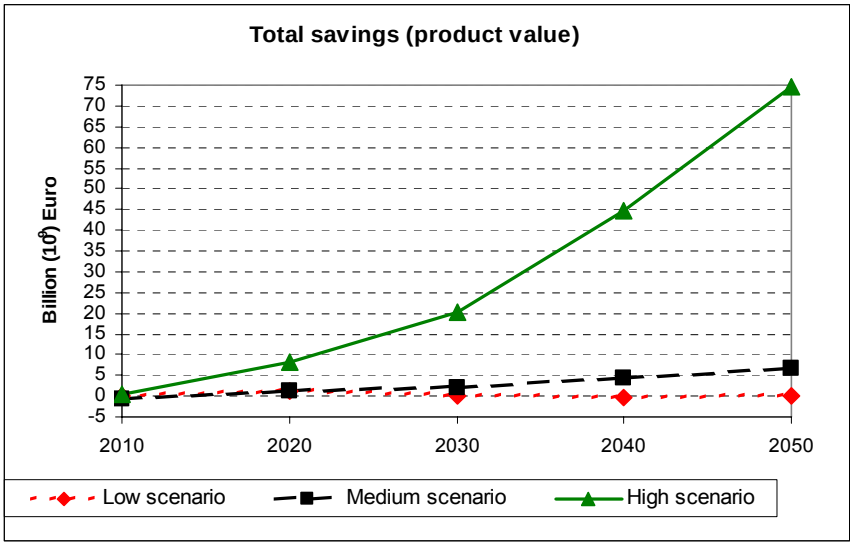

Figure 4-7: Total savings of product values by the production of bio-based chemicals in the different scenarios

The total non-renewable energy (NREU) savings and greenhouse gas (GHG) emission reductions that can be achieved by the production of bio-based chemicals in the different scenarios depend on the type of feedstock used. In general, energy savings and GHG emission reductions are higher if fermentable sugars from lignocellulose instead of fermentable sugars from starch are used.[79] Figure 4-8 shows, that energy savings and GHG emission reduction in the different scenarios are closely related. With regard to energy savings, we refer to *cradle-to-factory gate* non-renewable energy (NREU), while the GHG emission reductions refer to the system *cradle-to-grave GHG*. The relevance of the indicator *cradle-to-factory gate NREU* has been explained in detail in Section 3.4.2. For GHG emissions, this choice was made in order to capture the benefits of the embodied renewable carbon. This decision is justified in view of waste management legislation in the European Union, according to which synthetic organic compounds must not be landfilled, which means that the overwhelming share will be incinerated (the remainder is recycled).

[79] For a more detailed discussion of different feedstocks, see Section 3.4.1 to 3.4.4 of this report.

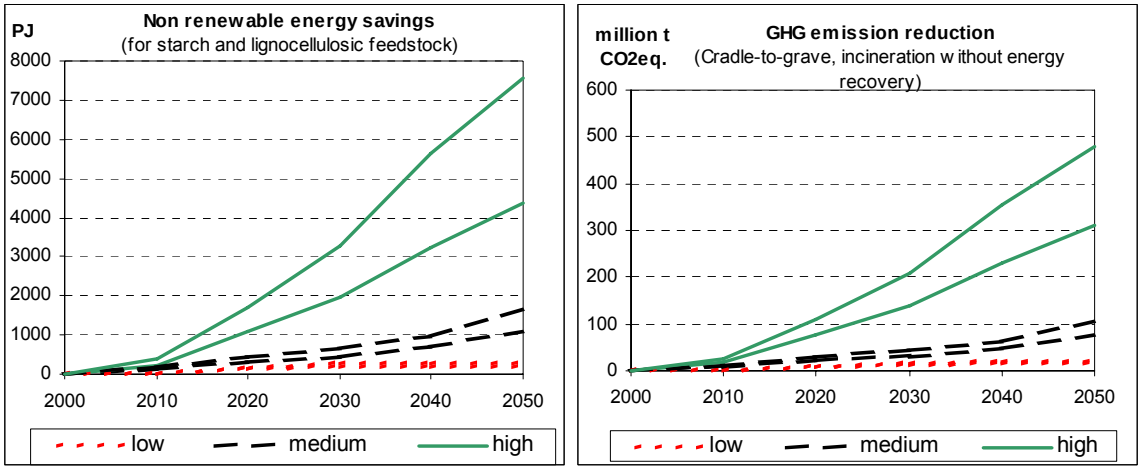

Figure 4-8: Non-renewable energy savings and GHG emission reduction in the three scenarios for lignocellulose and starch as a feedstock

In all scenarios, the production of bio-based chemicals leads to non-renewable energy savings as well as to GHG emission reductions. The total demand for non-renewable energy and the total GHG emissions of the chemical sector (under the condition that no bio-based chemicals are produced) depends strongly on the total demand for petrochemicals. The comparison can be made relative to the conventional *production of the selected chemicals* and relative to the conventional *total production of all organic chemicals* (compare Figure 4-5). In both cases, the energy demand and the greenhouse gas emissions of conventional production are calculated under the assumption of constant efficiencies (frozen efficiency and frozen structure):

- Compared to the *production of the selected chemicals* White Biotechnology allows to save about 7-10% of the energy demand (NREU) in the LOW scenario in 2050, while in the MEDIUM and HIGH scenario this percentage is about 20-30% and 39-67%, respectively (within each range, the lower value is for starch and the higher value for lignocellulosics; for all results by feedstock and year see Appendix A13).
- Instead of comparing the savings of energy and GHG emissions to the *production of the selected chemicals*, they can also be compared to the *total production of all organic chemicals*. For clarification: in our study we regard only a selection of possible bio-based chemicals and, thus, analyse only a fraction of the petrochemical market today: while in 2000 about 70 million tonnes of petrochemicals were produced (see Section 4.4.4), about 31 million tonnes (or about 50%) are within the scope of this analysis. Even though White Biotechnology chemicals might replace some of the excluded petrochemicals, we assume here that White Biotechnology does not offer any significant NREU and GHG savings in addition to those studied in Chapter 3 and included among the selected chemicals (Table 4-4). While this is a conservative assumption, it seems justified because i) the most promising White Biotechnology chemicals currently discussed have been taken into account, ii) the assumptions made in the Generic Approach represent upper limits (horizon values; see Section 3.1.1) and iii) no technological progress has been assumed for the production of petrochemicals (assuming technological progress would reduce the saving potentials).
  Dividing the NREU savings from White Biotechnology products by the NREU for the *total production of all organic chemicals* gives saving percentages for 2050 of 3-5% in the LOW scenario, 9-14% in the MEDIUM scenario and 18-32% in the HIGH scenario

(within each range, the lower value is for starch and the higher value for lignocellulosics; for all results by feedstock and year see Appendix A13). The lower saving percentages reflect the fact that the *total production of selected organic chemicals* is for all years around half of the *total production of all organic chemicals* (e.g., approx. 31 Mt versus 70 Mt in 2000).

In Table 4-8, the results for NREU savings are summarized for the three scenarios for year 2050. The importance of these savings relative to the total energy use of the entire economy will be discussed in Section 4.6.2.

	2000	2050		
		LOW	MEDIUM	HIGH
Production of ***all*** organic chemicals	[1]	[2]	[2]	[2]
- Production in million tonnes	~70	~70	~150	~300
- NREU for conventional production in EJ [3]	5.6	5.6	12.0	24.0
Production of ***selected*** organic chemicals (reference)				
- Production in million tonnes	31.0	31.0	65.3	135.9
- NREU for conventional production in EJ [4]	2.6	2.6	5.5	11.3
Starch-derived White Biotechnology products				
- Production in million tonnes	0	4.8	26.2	113.1
- NREU saved by White Biotechnology in EJ[5]	0.00	0.18	1.11	4.39
- NREU saved compared to ***selected*** chemicals in EJ[5]	0%	7%	20%	39%
- NREU saved compared to ***all*** organic chemicals in EJ[5]	0%	3%	9%	18%
Lignocellulosics-derived White Biotechnology products				
- Production in million tonnes	0	4.8	26.2	113.1
- NREU saved by White Biotechnology in EJ[5]	0.00	0.27	1.66	7.58
- NREU saved compared to ***selected*** chemicals in EJ[5]	0%	10%	30%	67%
- NREU saved compared to ***all*** organic chemicals in EJ[5]	0%	5%	14%	32%

1 EJ = 1 ExaJoule = 1000 PetaJoule = 10^{18} Joules

[1] See footnote in Section 4.4.4 for further explanations.

[2] Based on the assumptions for the growth rates of chemicals production in the scenario LOW (0% p.a.), MEDIUM (1.5% p.a) and HIGH (3% p.a.)

[3] An average NREU value for organic chemicals of 80 GJ/t has been assumed (this is somewhat lower than the overall weighted NREU value determined for polymers based on APME, var. years which yields a value of 88 GJ/t; compare also footnote No. 4). The value calculated in this manner for year 2000 (80 GJ/t multiplied with ~70 million tonnes production, i.e. 5.6 EJ as given in the table) represents 72% of the total energy use of the chemical industry (including process energy and feedstock energy) as reported in international energy statistics (IEA, 2003). The gap of 28% can be explained with the production of inorganic chemicals and other activities in the chemical industry (offices etc.).

[4] Calculated bottom-up by multiplication of the NREU of each chemical and weighted with its production share within the group of selected chemicals; this results in an overall weighted value of 74 GJ/t.

[5] All savings compared to petrochemical products assuming frozen technology and frozen structure

Table 4-8: Summary of the scenario results on savings of non-renewable energy (NREU) by White Biotechnology products in 2050

If White Biotechnology chemicals are produced in very large quantities land use could become a crucial factor but it remains relatively low in most *scenario*s. According to our calculations for the *production of the selected* chemicals fermentable sugar made of *starch* requires 1.0 to 38.2 million ha of land in 2050 in the three scenarios (Figure 4-9). If lignocellulose is used as bio-feedstock, only 0.4 to 15.6 million ha are needed (Figure 4-9).
These results discussed take into account that the production of bio-based chemicals in the scenarios is smaller than the production of the petrochemical products that serve as reference (16%, 40% and 83% in LOW, MEDIUM and HIGH; these percentages are calculated by dividing the production of bio-based chemicals by the *production of selected organic chemicals*; see Table 4-8). If we now assume that *selected organic chemicals* are *fully* substituted by White Biotechnology chemicals, the land requirements in 2050 in the three scenarios range between 17 and 63 million ha for starch and between 7 and 26 million ha for lignocellulosics. As third step we can make the hypothetical assumption that *all organic chemicals* (i.e. not only the selected ones; see Figure 4-5) are covered at 100% by White Biotechnology products; under these circumstances the land requirements would be about *twice as high,* i.e. reaching up to 126 million ha for starch and up to 52 million ha for lignocellulosics in 2050 (not shown in Figure 4-9). These results need to be compared to the availability of total agricultural land and of set-aside land. We will discuss this in Section. 4.6.2.

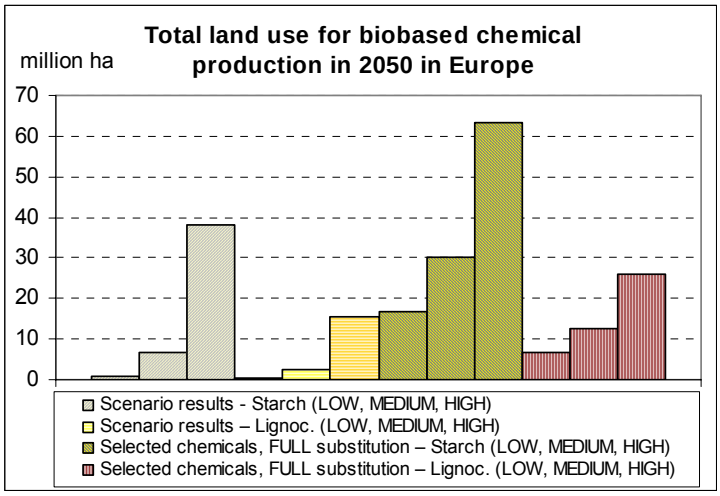

Figure 4-9: Total land used for the *selected organic chemicals* according to the three scenarios and for 100% bio-based chemical production (FULL substitution)

4.6 Discussion

4.6.1 Uncertainty and sensitivity

The market potentials in the LOW, MEDIUM and HIGH scenarios give an insight into the range of bio-based bulk chemical production that can be expected in the next decades. It should, however, be kept in mind that these scenario results are not projections of the future. First, the calculation of market potentials is based on parameters that are difficult to predict as, for example, fossil fuel prices. Second, the combination of parameters in the scenarios does not reflect any linkages. For example, a high demand of chemicals is not necessarily linked to a low sugar price in Europe (both are features of the scenario HIGH). Instead, the combination of the parameters chosen in the scenarios HIGH and LOW should result in the largest possible range of market potentials.

When relating the estimated savings to the total organic chemical industry we assumed above that there are *no significant savings due to White Biotechnology other than those studied in this report*. This concerns both other White Biotechnology products and other, more efficient process routes leading to the same products. Our arguments were that i) the most promising White Biotechnology chemicals have been taken into account, ii) the assumptions made in the Generic Approach represent upper limits (horizon values; see Section 3.1.1) and iii) no technological progress has been assumed for the production of petrochemicals. Moreover, a sugar price of 70 € /t (as assumed in the scenario HIGH) is likely to be too low for the long run (see below). We hence implicitly assume that these factors, which tend to lead to an overestimation of the saving potentials, compensate possible savings due to White Biotechnology products and processes, which have not been taken into account in this study. However, it needs to be emphasized that these assumptions are subject to uncertainty.

It should also be kept in mind that White Biotechnology is very likely to offer benefits also in the areas of fuels, food products and fine chemicals. These products are outside the scope of this project but would need to be included if we were to answer the question how large the *total* benefits of White Biotechnology are. The additional benefits due to *fuel only* can be expected to be rather large in view of the great market potential of ethanol in transportation.

Next, we discuss the uncertainties related to the key parameters of the scenario calculations. These are the level of fossil fuel prices, fermentable sugar prices, the development of production of the chemical sector as a whole and the importance of subsidies and the green premium in our model calculations:

- Future fossil fuel prices depend on (global) political developments as well as on the developments of reserves and demand. In the LOW scenario, a very moderate increase of fossil fuel prices has been assumed that concur with most studies (see Section 4.4.1). In the HIGH scenario, fossil fuel costs rise to up to 80 US$/barrel, which is rather high given most current estimates. However, even assuming very high fossil fuel prices of 105 US$/barrel in the HIGH scenario would lead to only slightly higher shares of bio-based bulk chemicals in 2050, i.e. 83.5% instead of 83%.
- It must be noted that we do not explicitly account for the effect of energy policy or of climate policy. The oil prices used in this study hence *implicitly include* the effects of

policy measures. A CO_2 tax of 10 €/t CO_2 translates to an equivalent of 4.6 US$/barrel.[80] For example, our maximum oil price of around 80 US$/barrel in 2050 in the HIGH scenario could hence be interpreted as a real oil price of 57 US$/barrel plus a CO_2 tax component of 23 US$/barrel (equivalent to 50 €/t CO_2).

- In several world regions, fermentable sugar is nowadays available at lower prices than in Europe. The difference is largest between Europe and sugar cane producing countries such as Brazil with a sugar price of 70 €/t (we have assumed this value in the scenario HIGH). Prices of sugar made from sugar cane are clearly higher in several other tropical countries because the wage level is higher (see Appendix A6). In the media (news/TV) in Western countries, it is being reported that the working and living conditions on Brazilian sugar cane plantations can be close to slavery and awareness on this issue is increasing in Brazil and in high-income countries. As a consequence of industrialization of the developing world and improved social standards, the wages and hence also sugar prices will converge to some extent across the globe. In 2050 there will most likely still be a gap in production cost for sugar across the world due to incomplete socio-economic convergence and for climatic and fertility reasons but the size of this gap is likely to be substantially smaller than today. The gradual decrease of the discrepancy in hourly labour cost across the globe will most likely have a stronger effect on labour intensive sugar cane production compared to exploitation and refining of crude oil which is not labour intensive. This point reinforces the hypothesis of a decreasing price gap between oil and fermentable sugar (ratio of the lowest sugar price worldwide to the oil price) and makes it also likely that the lowest sugar price worldwide will be larger than 70 €/t by 2050. In view of the socio-economic convergence, the calculated market potentials presented in this chapter for low sugar prices hence may be overestimated, i.e. the real market potentials of the bio-based bulk chemicals may be lower than calculated in our projections.
  With the increasing production and use of bioenergy (liquid biofuels and solid biofuels) the biomass prices are likely to become increasingly correlated to fossil fuel prices. This effect has already been visible in the recent past when the expansion of bioethanol in combination with high oil prices was accompanied by a rise in sugar prices (compare Appendix 6, Figure A6-1). To establish a quantitative relation between biomass prices (or sugar prices) and fossil fuel prices, a very comprehensive model would be required including the global and regional supply of agricultural and forest products and their use as wood for construction purposes, for bioenergy, chemicals, food and animal feed. Such a model is far beyond the scope of this project.
  While all these arguments speak for relatively higher biomass prices relative to fossil fuels one could also argue that oil prices may rise excessively due to surging demand especially from developing countries. The increase in oil price would then clearly outpace the rise in sugar prices. Under these conditions the market potentials for bio-based chemicals presented in this chapter could be clearly underestimated.
  To summarize, the development of sugar prices in the future remains unclear; however, the arguments speaking for rising sugar prices (and also for rising biomass prices) relative to the fossil fuel prices seem stronger.
- The fact that the further development of fermentable sugar prices is rather unclear for the next 50 years leads to substantial uncertainties for the final results of this study because the price level of fermentable sugar strongly influences the economics: for example, assuming a high sugar price of 400 €/t in the HIGH scenario, reduces the market potentials in 2050 to 37 million tonnes (instead of 113 million tonnes in the default case)

[80] Calculated assuming a CO_2 emission factor of 74 kg CO_2 /GJ (representative for oil products); 1 barrel (bbl) oil is equivalent to approx. 6.2 GJ (gross calorific value).

and assuming a low sugar price of 70 €/t in the LOW scenario, increases the market potentials to 8 million tonnes (instead of 5 million tonnes in the base case).

- It should also be noted that the market potentials of bio-based bulk chemicals are closely linked to the total production of chemicals because White Biotechnology (as any other new technology) is implemented more quickly in rapidly expanding markets compared to markets with slow or no growth. The total production of chemicals in Europe depends on overall economic growth, the structure of the economy and the industry and on the competitiveness of the European chemical industry. This competitiveness in turn may depend on the realization of White Biotechnology. In the three scenarios, we have assumed a very wide range of production values, reaching from 0% p.a. (physical) growth to 3% p.a. Therefore, the ratio of bio-based production relative to the total production of selected chemicals should also be taken into account as an important indicator.
- White Biotechnology might be stimulated by policy measures, e.g. subsidies (e.g. in the form of lower prices for industrial sugar or in the form of direct subsidies for the White Biotechnology sector, e.g. in the form of reduced VAT rates). Only in the HIGH scenario, moderate subsidies have been taken into account. Assuming a subsidy of 10% of the product value in the LOW scenario, leads to a 25% increase of the market potential in 2050. On the other hand, in the HIGH scenario the market potential only decreases by 0.1% if no subsidies are assumed. Therefore, especially under less favourable conditions for bio-based bulk chemicals, subsidies are desirable to stimulate the development of bio-based bulk chemical production.
- While subsidies have not been taken into account in the LOW and MEDIUM scenario, certain products are eligible to a "green premium" independently of the scenario studied (Table 4-4). Bio-based chemicals that are eligible to a "green premium" gain a limited market share even if their product value (i.e. the depreciated production cost) is larger than for its petrochemical equivalent. The "green premium" applies to all three scenarios. It explains partly why polylactic acid (PLA) is present in all three scenario projections (see Figure 4-5) while it was not found to be attractive in Chapter 3 for the techno-economic analyses assuming high fermentable sugar prices (Table 3-10). [81]

4.6.2 Putting the benefits into perspective

The achieved cost benefits highly depend on the total demand of chemicals and, thus, also depend on economic developments in Europe. By 2050, the total product value amounts to 6 to 103 billion € in the various scenarios, while the total sales of the chemical industry in the EU-25 were about 580 billion € and in the rest of Europe 60 billion € in 2004 (CEFIC 2005b). Of these sales, about 38%, i.e. 240 billion € were for bulk chemicals (in 2004). In view of the total product value savings discussed above (-0.13, 6.7 and 74.8 billion € depending on the scenario), we can conclude that White Biotechnology offers substantial product value savings in the HIGH scenario, while the savings are small in the MEDIUM scenario and the scenario LOW entails small additional expenses compared to the petrochemical benchmark. In the HIGH scenario, the economy's overall demand for chemicals can hence be satisfied at a much

[81] A further reason is that high oil prices make PLA economically viable compared to PET in the MEDIUM and HIGH scenario (economic viability without green premium and without subsidy).

lower overall cost. The resulting macroeconomic savings contribute to improved competitiveness.

For the annual added value of the bio-based chemicals, we calculated about 1.8, 8.8 and 33.2 billion € in the three scenarios in 2050. For 2010, our results range between 0 and 2.5 billion €. For comparison, Mc Kinsey estimates an added value of about 11 to 22 billion € by 2010 for the total of White and Red Biotechnology. In contrast to our calculations the value estimated by Mc Kinsey includes fine chemicals and pharmaceuticals and also enzymatically produced chemicals, which have a large potential compared to fermentation based bulk chemicals especially on the short term (EuropaBio 2003).

It should also be noted, that no technological developments in the petrochemical industry have been taken into account in this study since it was beyond the scope of this study to analyse also the improvement potentials for conventional processes; since we anyway expect only a relatively small technological progress for petrochemical processes, this assumption should not lead to any major bias in the conclusions. However, including the technological progress in petrochemical processes would lead to smaller benefits of White Biotechnology than discussed here.

In order to put the NREU savings into perspective we compared in Section 4.5.2 the NREU savings due to White Biotechnology firstly to the energy use of the *production of the selected chemicals* and secondly to the *total production of all organic chemicals*. Covering all results (all three scenarios for starch and for lignocellulosics) we found saving potentials between 7% and 67% in the first case and between 3% and 32% in the second case. Today, the NREU (including primary energy equivalents of power production) of the total chemical industry in OECD Europe represents around 9.5% of the total energy (total primary energy supply) in all OECD Europe countries. Under the assumption that the importance of energy use in the chemical sector will not change decisively in the decades to come we can multiply this share (9.5%) with the saving percentages for the second case (between 3% and 32%). We hence estimate that White Biotechnology chemicals allow to save in 2050 0.3% to 3.0% of the non-renewable energy use (NREU) of the entire economy in 2050 (the range covers all three scenarios for starch and for lignocellulosics).[82] The saving percentages for GHG emissions are in a similar range.[83] We conclude that the savings are limited at the macroeconomic scale (because the chemical sector represents only roughy 10% of the total economy's energy use) but can be substantial at the level of the chemical industry (up to 32% in the scenario HIGH).

In Section 4.5.2 we presented the results for land use assuming three different levels of substitution. We now first discuss the *production of the selected chemicals according to the scenario analyses* and then secondly deal with the extreme case of manufacturing *all organic chemicals* by White Biotechnology. In the first case 1.0 to 38.2 million ha of land are required

[82] These percentages are confirmed if we relate our projections for energy savings by White Biotechnology to projections for energy use in OECD Europe as prepared by the IEA. The primary energy use in OECD Europe in 2000 was around 74 EJ and based on the outcome of several models a demand of 86 EJ can be expected for 2030 and of 96 EJ for 2050 Compared to these values our scenario calculations for non-renewable energy savings by bio-based bulk chemical production are limited, with 0.2 to 2.0-3.3 EJ (low value for starch, high value for lignocellulosics) or 0.2% to 2.3-3.8% in 2030 (and 0.2 to 4.4-7.6 EJ or 0.2% to 4.6-7.9% in 2050).

[83] In the SRES marker scenarios of the IPCC, about 7 to 18 Gt CO_2 are emitted from fossil fuels and industrial sources in the whole OECD in 2050. In 2000, about 31% of OECD CO_2 emissions are emitted in OECD Europe. (IEA 2002). Multiplication of this percentage with the emissions in the OECD according to the IPCC scenarios results in an estimate of about 2 to 6 Gt CO_2 for OECD Europe in 2050. In comparison, GHG emission reductions of between 0.01 and 0.31-0.48 Gt CO_2 by White Biotechnology chemicals according to our calculations (the range covers all three scenarios for starch and for lignocellulosics) are limited.

in 2050 if starch is used and 0.4 to 15.6 million ha are needed if lignocellulose is chosen (ranges cover all three scenarios). In the second case land requirements in 2050 reach up to 126 million ha for starch and up to 52 million ha for lignocellulosics.

For comparison, the agricultural area in the EU-25 was about 179 million ha in 2002 (FAO 2005). A more relevant basis for comparison is the available surplus of agricultural land for food production. It is estimated that by 2010 15% of arable farmland in the EU-15 can be set aside (amounting to 15-20 million ha), while later in the 21st century even more than 50 million ha can possibly be set aside (Rogner 2000). Assuming the same percentages, about 27 million ha can be set-aside in 2010 and 77 million ha later in the 21st century in the EU-25. Due to the current low agriculture yields in Central Eastern Europe, the potential is probably even larger in the long term for the EU-25. The land requirements for our first case, i.e. the *production of the selected chemicals according to the scenario analyses*, are clearly lower: In the most land intensive case (starch, scenario HIGH) a maximum of 1.8 million ha and 38.2 million ha is used in 2010 and 2050 respectively. In contrast, the production of *all organic chemicals* by White Biotechnology is not feasible if starch is used as feedstock (126 million ha would be required in 2050) and about two thirds of the set-aside land would be needed if lignocellulose is used (52 million ha in 2050). However, part of the available agricultural land will be used for the production of bioenergy. Moreover, bio-based chemicals can be produced not only by White Biotechnology but also i) by direct use of compounds found in nature and their modification (e.g., use of starch to produce thermoplastic starch) and ii) by thermochemical conversion processes. On the other hand, the transition to lignocellulosics as feedstock would open up the possibility of using woody biomass not only from agricultural land but also from forests. Therefore, an in-depth analysis of the land use competition between bioenergy and chemicals would be required in order to evaluate the upper limit for the production of bio-based bulk chemicals. It is expected that the *production of the selected chemicals* is, *in general*, feasible from a land availability point of view but that the production from starch in the scenario HIGH from 2040 onwards could face some limitations.

4.7 Conclusions

The scenario analysis presented in this chapter yields a broad range of values for the possible market development of White Biotechnology chemicals. In the LOW scenario, which can be seen as the lower limit for bio-based chemical production, the share of White Biotechnology chemicals relative to all organic chemicals (70 Mt in 2050; see Section 4.4.4 and Figure 4-5) is about 7% (or 5 million tonnes) in 2050 (see Figure 4-5 and Table 4-8). In the HIGH scenario representing the upper limit of bio-based chemical production under very favourable conditions and a total production of all organic chemicals of around 300 Mt in 2050, this share is about 38% (or 113 million tonnes). Compared to these two extremes, the MEDIUM scenario represents a more probable future trajectory resulting in shares of 17.5% (or 26 million tonnes) in 2050. Although the MEDIUM scenario is probably the most realistic in terms of production volumes for the chemical sector as a whole, this scenario should

nevertheless not be chosen as reference case; the main reason is that the development of chemical demands, oil prices, sugar prices and supportive policies are uncertain. [84]

A key criterion for the preselection of the bio-based chemicals studied in the scenario analysis is the large economic potential. Of the preselected chemicals, PLA, PHA and PTT have large market potentials even at less favourable conditions. n-Butanol, succinic acid and ethyl lactate become interesting in terms of market potentials at intermediate conditions, while ethylene and adipic acid require favourable to very favourable conditions. Acetic acid has low market potentials under all conditions.

Concerning environmental benefits we have estimated that White Biotechnology chemicals allow to save in 2050 0.3% to 3.0% of the non-renewable energy use (NREU) of the entire economy (the range covers all three scenarios for starch and for lignocellulosics). The saving percentages for GHG emissions are in a similar range. We conclude that the savings are limited at the macroeconomic scale. This is not amazing because the NREU (including primary energy equivalents of power production) of the total chemical industry in OECD Europe is around 9.5% of the total energy (total primary energy supply) of the entire economy.

It is therefore more adequate to perform the comparison at the level of the chemical industry. Compared to the conventional production of all organic chemicals, White Biotechnology allows to save 3-5% energy in the LOW scenario, 9-14% in the MEDIUM scenario and 18-32% in the HIGH scenario (lower value for starch; higher value for lignocellulosics; percentages relative to *all organic chemicals*; see Table 4-8). Hence, White Biotechnology allows to achieve substantial savings at the level of the chemical industry (up to 32% in the scenario HIGH).

A precondition for the development of White Biotechnology for chemicals is the availability of bio-based feedstock. Land use was not found to be a bottleneck for Europe (EU-25) for a pathway between the MEDIUM and the HIGH scenario, especially if the use of lignocellulosic feedstocks is successfully developed.

With regard to economics, especially the HIGH scenario offers considerable product value savings 74.8 billion € which contribute to improved competitiveness. Under these conditions a clear win-win-situation is achieved by combination of substantial economic and environmental benefits. Also the MEDIUM scenario is accompanied by economic benefits (6.7 billion € product value savings) even though these are considerably lower.

If Europe decides to seriously pursue White Biotechnology chemicals, then a pathway between the scenarios MEDIUM and HIGH should be sought for in order to obtain meaningful savings for energy and GHG emissions while achieving substantial economic benefits. In terms of not only energy use and GHG emissions but also land use and feedstock availability, the use of lignocellulosics as basis for fermentable sugar is highly recommended. According to our calculations for the MEDIUM and HIGH scenario, the use of lignocellulosics allows NREU savings of 14%-32% in 2050 (percentages relative to *all organic chemicals*; see Table 4-8). These are respectable savings if one considers that they are

[84] For example, higher oil prices than those presumed in the MEDIUM scenario (beyond the 66 US$/barrel in 2050), lower sugar prices (e.g. 135 €/t instead of 200 €/t in MEDIUM) and proactive R&D enabling earlier adoption of advanced technologies (around 2020 instead of 2040 in MEDIUM) can move the saving potentials in direction of the values calculated for the HIGH scenario.

achieved among the White Biotechnology chemicals representing not more than 17% (MEDIUM scenario) and 36% (HIGH scenarioof *all organic chemicals* (32% NREU savings between the years 2000 and 2050 is equivalent to average yearly savings of 0.77%[85] over 50 years).

These substantial energy savings and GHG emission reduction by White Biotechnology for bulk chemical production may become increasingly important as the improvement potentials in conventional processes are more and more exploited (parallel to the increasing maturity of petrochemical industry and as a consequence of the sharp decline in R&D in this sector).

Petrochemical feedstock prices as well as fermentable sugar prices are decisive for the market potentials of bio-based chemicals. The large range of results reflects the uncertainties around the development of parameters. Technological developments in White Biotechnology are also influencing the market potentials strongly. Therefore, high and economically favourable market potentials of bio-based chemicals in Europe are possible only if technological developments in biotechnological processes proceed, bio-feedstock costs are lower than current sugar prices and fossil fuel prices increase. European policy to stimulate the introduction of bio-based chemicals would therefore have to aim to decrease sugar prices and to favour technological development. Supportive measures to shorten the adoption process would also be highly desirable.

[85] Calculation: $1 - (100\% - 32\%)^{1/50} = 0.77\%$ p.a.

5. Risks of White Biotechnology in perspective[86]

In this chapter, we discuss the *risks* related to products of White Biotechnology in comparison with conventional chemical products derived from fossil fuels. A risk is generally defined as "the quantitative or qualitative expression of a possible loss that considers both the probability that a hazard will happen and the damage caused by the event" (ES&H manual, not dated). The concept of risks thus contains the elements "chance" (probability) and "consequences". Klinke and Renn (2002) developed a classification for risks that is based on differences in chance and consequence of risks. They use Greek mythology to classify the risks. An overview is given in Table 5-1.

Risk class	Probability	Magnitude	Other criteria	Typical examples
Damocles	low	high	not decisive	nuclear energy, dams, large-scale chemical facilities
Cyclops	uncertain	high	not decisive	nuclear early warning systems, earthquakes, volcanic eruptions, AIDS
Pythia	uncertain	uncertain	not decisive	greenhouse effect, BSE, genetic engineering
Pandora	uncertain	uncertain	high persistency	POPs, endocrine disruptors
Cassandra	high	high	high delay	anthropogenic climate change, destabilization of terrestric ecosystems
Medusa	low	low	high mobilization	electromagnetic fields

Table 5-1: Overview of the risk classes, their criteria and typical representatives

The assignment of a given technology or case to a risk class depends on the assessment of both the probability and the magnitude of the risk (see Table 5-1). Technologies or cases characterized by large (information-) knowledge gaps qualify for the risk classes "Pythia" and "Pandora". If increasing insight reduces the uncertainties, one of the other risk classes may be more representative for the case studied. However, in spite of the enhanced knowledge, considerable room for subjective assessments might still remain. Large knowledge gaps currently exist for the biotechnological production of bulk chemicals (including both White Biotechnology and the production of chemicals in genetically modified crops), potentially leading to a wide range of subjective valuations and conclusions. While there might be sufficient evidence to exclude the risk classes "Damocles" and "Pandora", all other classes do seem eligible depending on the concrete product and process studied.

This chapter deals with both *conventional* risks related to White Biotechnology (Section 5.1) and with risks related to genetically modified (GM) microorganisms and crop plants (Section 5.2). We finally draw our conclusions in Section 5.3.**Conventional risks**

In this chapter we develop and apply a generic approachfor the risk assessment of petrochemicals and bio-based chemicals, thereby focussing on *conventional risks*. With *conventional risks* we refer to risks to human health and life, thereby taking into account accidents, illnesses and external risks imposed on the public due to emissions and

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technological disasters. Five cases are studied, i.e. PTT, PHA, PET, PE and ethanol. The approach combines rather classical risk assessment methods (largely based on chemistry) as developed by the Life Cycle Assessment (LCA) community with statistical information on technological disasters, accidents and work-related illnesses. The method covers the *total process chain* for petrochemical and bio-based products *from cradle to grave*.

5.1.1 Methodology

This paragraph explains the methodology applied for the comparative risk assessment of bio-based chemicals and petrochemical products. The method is generic in the sense that it is based on risk relationships for representative cases and allows to make a first estimate of the total risk of a given process chain (system) leading to a given chemical. The process chain encompasses the entire life cycle from "cradle" to "grave" and therefore covers the following six sectors:

- Agriculture
- Extraction and refining of fossil fuels
- Chemical industry
- Power generation
- Transport
- Waste management

We limit the analysis to the risks to human health, while risks to the environment are not taken into account due to incomplete information (see below). We estimate the total risk to human health throughout the life cycle by adding up the results for the following four risk categories:

- External risks (risks imposed on the public) due to *regular* release of emissions
- External risks due to technological disasters
- Risks of work-related accidents
- Risks of work-related illnesses.

Theoretically, a similar method could be devised for risks to the environment. In particular, the methodology developed below for health risks caused by the *regular* release of emissions could, in principle, be transferred to environmental risks. However, firstly, certain external risks caused by *regular emissions* - especially the loss of biodiversity - cannot be quantified due to the lack of data and because internationally accepted methods do not exist so far. And secondly, information on the impacts of *technological disasters* to the environment is largely missing. For these reasons this chapter focuses on the risks to human health while excluding environmental risks.
The risk assessment is conducted as follows: For each of the four risk categories listed above, we first estimate the total risk of each of the six sectors listed above (agriculture etc.) for Western Europe as a whole. We then divide these totals by suitable reference units, which are given in Table 5-2. This leads to a matrix with specific risk indicators. Multiplication with the respective reference flows of the given process chain (system) and addition of the intermediate results leads to a generic assessment of the overall risk. The objective of the next sections (Section 5.1.1.1 to 5.1.1.5) is to explain the development of the risk matrix. Next, we explain the approaches devised for the four risk categories listed above.

Sector	Reference unit
Agriculture	TJ crop output
Extraction and refining of fossil fuels	TJ crude oil consumption
Chemical industry	TJ fossil feedstock consumption
Power generation	TJ electricity output
Transport	tkm road and rail freight transport
Waste management	TJ incinerated waste

Table 5-2: Reference units per sector (Abbreviations: TJ = Terajoule; tkm = ton-kilometre)

5.1.1.1 External risks due to regular release of emissions

We base the quantification of the risks to human health on the EPS 2000 method (Steen 1999), which is a "single-score method" developed for life-cycle impact assessment. "Single score" means that the various impact categories (e.g., human toxicity, climate change, acidification etc.) are aggregated to one single indicator by means of weighting factors. The outcome is hence one single value for a given case. In the case of the EPS 2000 method, the number of "personyears"[87] lost is the common indicator to measure impacts on human health (other methods use, for example, dimensionless metrics or "external costs"). The EPS methodology incorporates estimates of the hazard (damage potential) and the probability of its occurrence and is therefore a metric for the risk to human health. The following five categories for impacts to human health are distinguished:

- Life expectancy: This is defined as years of lost life (YOLL).
- Severe morbidity and suffering: This is defined as the time that a human suffers severe morbidity including starvation.
- Morbidity: This is defined as the time a person suffers morbidity like a cold or flue.
- Severe nuisance: This is severe nuisance that would normally cause a reaction to avoid the nuisance.
- Nuisance: This is nuisance that is irritating but not causing any direct action.

In the EPS methodology these categories are weighted differently (see Table 5-3). The division of each weighting factor by the weighting factor of the category "life expectancy" enables us to express all categories in terms of personyears of life lost (YOLL). This is the unit that is used to quantify the risks for all inputs in this risk assessment.

Human health impact category	Weighting factor (Environmental load units *) per personyear)	Weighting factor normalized to "life expectancy"
Life expectancy	85000	1
Severe morbidity	100000	1.1765
Morbidity	10000	0.11765
Severe nuisance	10000	0.11765
Nuisance	100	0.0011765

*) 'Environmental load units' are used by the EPS method to express final environmental impacts.

Table 5-3: Categories for impacts on human health and their weighting factors according to the EPS 2000 method (Steen 1999)

[87] A personyear represents suffering of one person during one year.

For each sector, the risks according to EPS 2000 are calculated by use of the LCA tool Simapro 6 (PRé Consultants 2004).

For *agriculture* the risks (in YOLL) are calculated per TJ of crop output (as shown in Table 5-2). The chosen crop for our calculations is maize because this is the feedstock we assume for bio-based production of PTT, PHA and ethanol, which will serve as cases for application of the risk assessment (Section 5.1.2).[88] For the *extraction and refining of fossil fuels* the total emissions of the sector "mineral oil and gas refineries" in EU-15 countries were used (Brand et al. 2004). After having calculated the risks of these emissions to human health (by use of the EPS 2002 method) the results were divided by the total crude oil consumption of petroleum refineries in the EU in 2000 (approx. 28,200 PJ according to IEA, 2002).[89] For the *chemical industry* the same approach was chosen as for extraction and refining of fossil fuels. Total emissions of the sector "basic organic chemicals" in EU-15 countries are taken from Brand et al. (2004). The result according to the EPS 2000 method is divided by the total petroleum product feedstock consumption of the chemical and petrochemical industry in the EU in 2000 (approx. 2,700 PJ according to IEA 2002).[90] For *power generation* we used the EPS 2000 method to calculate the impacts related to 1 TJ of electricity (weighted electricity mix of the UCTE-, CENTREL- and NORDEL grid).[91] For *transport* it is assumed that all transport takes place with a 32 tonne-load-capacity lorry.[92] Finally, for *waste management* we apply the EPS method to calculate the impacts for the incineration of 1 TJ of polyethylene terephtalate (PET) (HHV = 23.13 GJ/tonne).[93] It is assumed that this process can be applied to other plastics (PTT, PHA and PE) and ethanol as well. During the incineration of PET, electricity and heat are produced.[94] To account for the avoided conventional production of electricity and heat (in the form of steam), the respective impacts are subtracted (credit approach).

5.1.1.2 External risks due to technological disasters

Technological disasters with fatalities seem to be relatively rare (UNEP 2001). In readily available overviews on disasters, no distinction is made between fatalities among employees on the production site ("on site") and citizens outside the production site where the disaster took place (Kleiber 2004). It is therefore difficult to quantify external risks due to

[88] The exact name of the chosen product in Simapro 6 is "grain maize IP, at farm/CH S". IP = Integrated production, CH = Switzerland, S =System. The calorific value of maize is 14.9 GJ/tonne.

[89] This value is also used as reference for the risks due to accidents and illnesses discussed in Section 5.1.1.3 and 5.1.1.4.

[90] This value is also used as reference for the risks due to accidents and illnesses discussed in Section 5.1.1.3 and 5.1.1.4.

[91] The categories chosen in Simapro are

- Electricity, medium voltage, production UCTE, at grid/UCTE S
- Electricity, medium voltage, production CENTREL, at grid/CENTREL S
- Electricity, medium voltage, production NORDEL, at grid/NORDEL S

The three categories were weighted according to their production shares, i.e. 74% UCTE, 11% CENTREL and 15% NORDEL (Frischknecht and Faist Emmenegger 2003).

[92] The exact name of the chosen product in Simapro 6 is "Transport, lorry 32 t/RER S".

[93] The exact name of the chosen product in Simapro 6 is "Disposal, polyethylene terephtalate, 0.2% water, to municipal incineration/CH S".

[94] During the incineration of 1 TJ PET, 0.106 TJ electricity is obtained and 0.217 TJ heat. It is assumed that the heat is obtained in the form of steam. Impacts are calculated in Simapro from electricity similar as was done in the section "power generation" and from steam using the Simapro category "Steam, for chemical processes, at plant, RER S"

technological disasters. An attempt is made here: In the last two decades only two major technological disasters are reported by UNEP (2001) in the industrial sector in Europe:

- Enschede, the Netherlands, 13 May 2000: explosion of a fireworks factory, 20 fatalities in total
- Toulouse, France, 21 September 2001: ammonium nitrate explosion in fertiliser factory: 7 fatalities outside the production site

This amounts to 27 fatalities among citizens in Europe in twenty years (on average 1.35 fatalities per year).

For the industrial sector in the EU, the European Environmental Agency (EEA 2001) reports 16 technological disasters between 1984 and 1996 with fatalities outside the production site and 47 technological disasters with fatalities on site. The occurrence of technological disasters with fatalities outside the production site is hence around one third of the value on the production site. No quantitative information is given on the number of fatalities (number of deaths). We therefore use the abovementioned values on the occurrence of technological disasters to estimate roughly the distribution of fatalities on site and outside the production facility. Multiplication of the reported 57 work-related fatal accidents in the chemical industry in 1999 (European Communities 2002) with 1/3 leads to the rough estimate of around 20 fatalities per year outside the production site (external risks). This is a rather high value compared to the fatalities in the last two decades reported above (27 in Enschede and Toulouse).

Combining the two approaches (direct deduction from the number of events in the last two decades versus combined use of statistical data) we conclude that the number of fatalities outside the production site due to technological disasters in the chemical industry is between 1 and 20 per year in Western Europe.

5.1.1.3 Accidents

We take into account two types of accidents in our risk assessment: fatal accidents and accidents with more than three days absence. In order to convert data on the occurrence of accidents (data for 1999 from European Communities 2004) into personyears of life lost (YOLL) several assumptions need to be made which are subject to substantial uncertainties. We account for these uncertainties in an uncertainty analysis (see below).

Fatal accidents

For fatal accidents it has to be determined how many years of life are lost. This is estimated by assuming the average age at which the accident occurs and estimating the years of life lost (YOLL) by comparison with the average life expectancy.[95] By subtracting the two values we arrive at the estimate that one fatal accident is equivalent to 34.75 YOLL.

[95] The following assumptions/estimates are made:

- We assume firstly that workers are employed from the age of 20 to 65 years and secondly that there is a uniform probability of a fatal accident during this period. The average age at which the fatal accident occurs is then estimated to be 42.5.
- Life expectancy for EU-15 in 2002 is 75.8 years for males and 81.6 years for females (Federal statistical office Germany 2004)
- In industry the majority of the workers is male. According to North Yorkshire County Council (2001) 75% of the workers in manufacturing are male. This brings the average life expectancy to (0.75 x 75.8 + 0.25 x 81.6 =) 77.25 years.

Accidents > 3 days absence
For accidents leading to over three days absence from work we assume that the EPS category "morbidity" applies which is equivalent to 0.11765 YOLL (compare Table 5-2). We estimate the average period of absence from work by use of another data source (European Agency for Safety and Health at Work 2002) and arrive at 30 lost working days.[96] We finally conclude that one accident of this type is equivalent to 0.0136 YOLL.[97]

Data on the occurrence of accidents are available for five of six sectors[98] that are relevant for our risk analysis (data from European Communities 2004). After having used these data to estimate YOLL we determine specific values by division by the activity level in the respective sector.[99]

5.1.1.4 Work-related illnesses

Among the work-related illnesses (reported by European communities 2004), two types are considered to be relevant for this risk assessment, i.e. pulmonary health problems and musculoskeletal health problems.[100] The data on prevalence of the health problems are converted to person years of life lost.

Pulmonary health problems
We assume pulmonary health problems to fall under the category "morbidity" (compare Table 5-3). Some of the occupational respiratory diseases take several decades to develop (e.g., respiratory cancer, asbestosis and silicosis) and quite often they become apparent only after retirement (European Communities 2004). It is therefore assumed that the period of

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- A fatal accident thus reduces on the average a life period from 77.25 years to 42.5 years. These are 34.75 years of lost life (YOLL).

[96] According to the European Agency for Safety and Health at Work (2002) every year nearly 5 million employees in the EU suffer from work-related accidents involving more than three days absence from work and a further 5500 are killed. As a result of this 150 million workdays are lost. Due to lack of more detailed data we make the simplifying assumption that all workdays are lost due to accidents involving more than three days absence from work. One accident involving one employee causes 30 lost working days (= 150 million/ 5 million).

[97] With 260 working days in a year, one accident causes 30/260 = 0.115 year of morbidity. Multiplication with the weighting factor of 0.11765 according to Table 5-2 gives a value of 0.0136 YOLL.

[98] Data on accidents are not available for waste management.
[99] The following data were used as a proxy for the activity level in the various sectors:
- For agriculture the total crop production in the EU-15 countries amounted to in 1999 was 4520 TJ in 1999 (FAO 2004).
- For extraction and refining of fossil fuels, see text on External risks.
- For chemical industry, see text on External risks.
- For power generation, the total amount of electricity generated by electricity plants and CHP plants in EU-15 in the year 2000 is used as reference (9,200 PJ according to IEA 2002).
- For transport, road freight transport (1320 Gtkm) and rail freight transport (240 Gtkm) add up to 1560 Gtkm.
- For waste management, only emission data are available that are already expressed per TJ waste.

[100] We did not take into consideration the category "Stress, depression or anxiety" (European communities 2004).

suffering a pulmonary health problem is 10 years at maximum. This leads to a value of 1.1765 YOLL per pulmonary health problem.

Musculoskeletal health problems
As for pulmonary health problems, we consider musculoskeletal health problems to fall under the category "morbidity". Using additional data for the United Kingdom, we estimate one case of muscoskeletal health problems to represent 0.004525 YOLL.[101]

5.1.1.5 Risk indicator matrix

Combination of the data discussed above leads to the risk indicator matrix shown in Table 5-4, which forms the basis for the risk assessment in this study. In some cases different sources from different years provide different data on accidents, which results in a data range. Table 5-4 shows only average values.

All values in YOLL	Reference unit	Regular emissions	Fatal accidents	Accidents >3days absence	Pulmonary health problems	Musculoskeletal health problems	Total
Agriculture	1 TJ crop output	-0.0321	5.11E-3	1.06E-3	5.01E-3	1.48E-4	-0.0208
Extraction and refining of fossil fuels	1 TJ crude oil consumption	0.00716	8.18E-6	7.08E-7	2.47E-5	6.88E-7	0.00719
Chemical industry	1 TJ fossil feedstock comsumption	0.0372	5.72E-4	2.18E-4	0.003	8.49E-5	0.0411
Power generation	1 TJ electricity output	0.245	1.26E-4	1.86E-5	3.2E-4	9.19E-6	0.245
Transport	1 tkm road and rail freight transport	3.48E-7	1.11E-8	2.7E-9	4.46E-9	2.89E-10	3.67E-7
Waste management	1 TJ incinerated waste	0.0517	-	-	-	-	0.0517

Table 5-4: Risk indicator matrix in "years of lost life" (YOLL) expressed per reference unit

5.1.2 Results

Applying the risk assessment method described above to the chosen cases results in an amount of YOLL per unit of product throughout the process chain. The final results are shown in Table 5-5 for PTT, PHA, PET, PE and ethanol. In Figure 5-1 to 5-6 the results are shown graphically.

According to the results shown in Figure 5-1 to 5-6 the conventional risks of all bio-based products studied are lower than for the petrochemical products: For PTT the risk of the bio-based production is 12-25% lower compared to petrochemical production. The risk of the production of PHA by fermentation was found to be 7-22% lower than the risk of the production of PET. For PHA and PE the difference is 39-49%. For ethanol the risk of the

[101] According to the University of Edinburgh (not dated) there are 1.2 million work-related musculoskeletal health problems in the UK. According to Unison (2002) 12.3 million working days are lost in the UK due to musculoskeletal health problems. This means that 1 musculoskeletal health problem causes on average 10 working days of absence. There are 260 working days in a year, which means that 1 musculoskeletal health problem is 0.0384 personyear of "morbidity". Multiplication with the conversion factor according to Table 5-2 this gives 0.004525 YOLL.

production by dry milling is 68-74% lower compared to the production from ethylene. While these results seem to justify the conclusion that the risks related to bio-based products are lower than for petrochemical products, it is indispensable to account for the uncertainties of the method applied before drawing final conclusions. An uncertainty analysis is therefore conducted in Section 4 (see below).

By far the most important source of risks (expressed in terms of Years of Lost Life, YOLL) are external risks due to the regular release of emissions to the atmosphere, followed by pulmonary health problems of workforce and accidents of the workforce (fatal accidents and accidents with more than three days of absence). External risks imposed on the public due to technological disasters are found to be negligible.

The results allow to compare how the risks are distributed over risk categories and industrial activities. The following conclusions can be drawn: The largest difference between bio-based and petrochemical products concerns risks related to the regular release of emissions to the atmosphere. Pulmonary health problems and fatal accidents tend to be more important for bio-based polymers than for petrochemical products but these differences are by far overcompensated by risks caused by the regular release of emissions to the atmosphere.
The split of the total risk by sector included in the process chain shows that the chemical industry is more important for the petrochemical products than for bio-based products. Waste management also plays an important to very important role. The contribution of waste management is equal for all production routes (petrochemical and bio-based) because it is based on the calorific value of the product. Transport is equal for bio-based and petrochemical production because equal transport is assumed for all production routes (500 tkm by 32 tonne-load-capacity-lorry). The sector agriculture is only of relevance for bio-based production routes. Cultivation of crops yields a "negative risk" in the sector agriculture, which is due to the uptake by crops of CO_2 from the air (CO_2 uptake is valued as a negative impact by the EPS 2000 method). It should, however, be noted that the experience made with soy bean production in Argentina shows that the large-scale cultivation in monocultures can result in serious impacts for the environment and for human health (Joensen et al., 2005). The share of the sector "extraction and refining of fossil fuels" tends to be slightly higher for petrochemical production routes. The sector "power generation" seems more or less of equal share in bio-based and petrochemical production of PTT. For PHA it is higher compared to PET and PE. For the production of ethanol, the share of "power generation" is very small to negligible in all cases.

Product/process	Abbreviation	**Risk (YOLL/tonne)**
PTT		
- from ethylene oxide	EthOx	0.003821
- from acrolein	Acr	0.004031
- via anaerobic fermentation on dextrose	Anaer/dextr	0.003001
- via anaerobic fermentation on glycerol	Anaer/glyc	0.003227
- via aerobic fermentation 1	Aer 1	0.003039
- via aerobic fermentation 2	Aer 2	0.003381
PHA		
- via fermentation 1	PHA 1	0.002501
- via fermenation 2	PHA 2	0.002988
PET	PET	0.003211
PE	PE	0.004949
Ethanol		
- from ethylene	from ethylene	0.003535
- via maize dry milling 1 (low estimate)	dry milling 1	0.000934
- via maize dry milling 2 (high estimate)	dry milling 2	0.001114

Table 5-5: Results of the risk assessment for PTT, PHA, PET, PE and ethanol

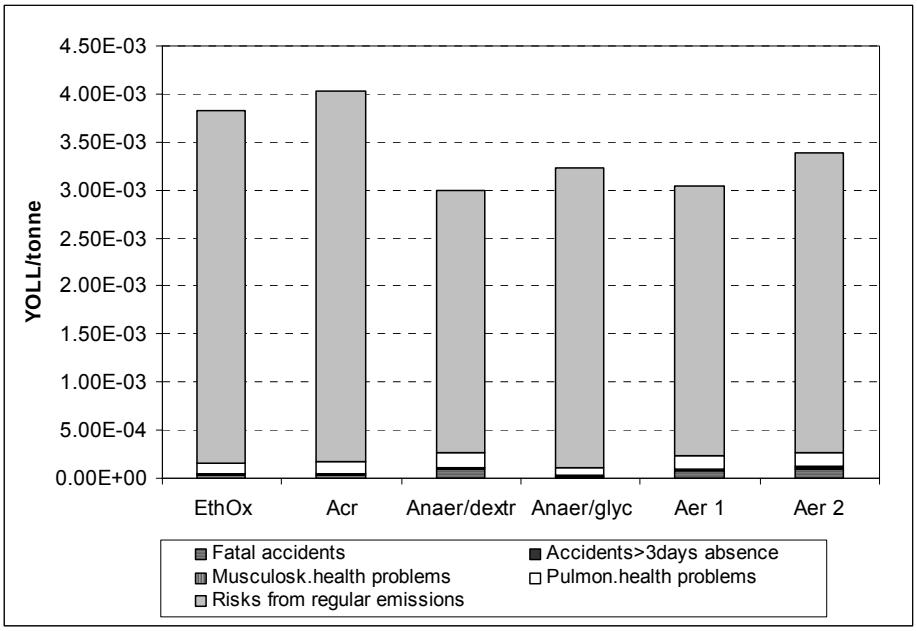


Figure 5-1: Results for PTT showing relative contributions of the different factors (for abbreviations on the x-axis see second column in Table 5-5)

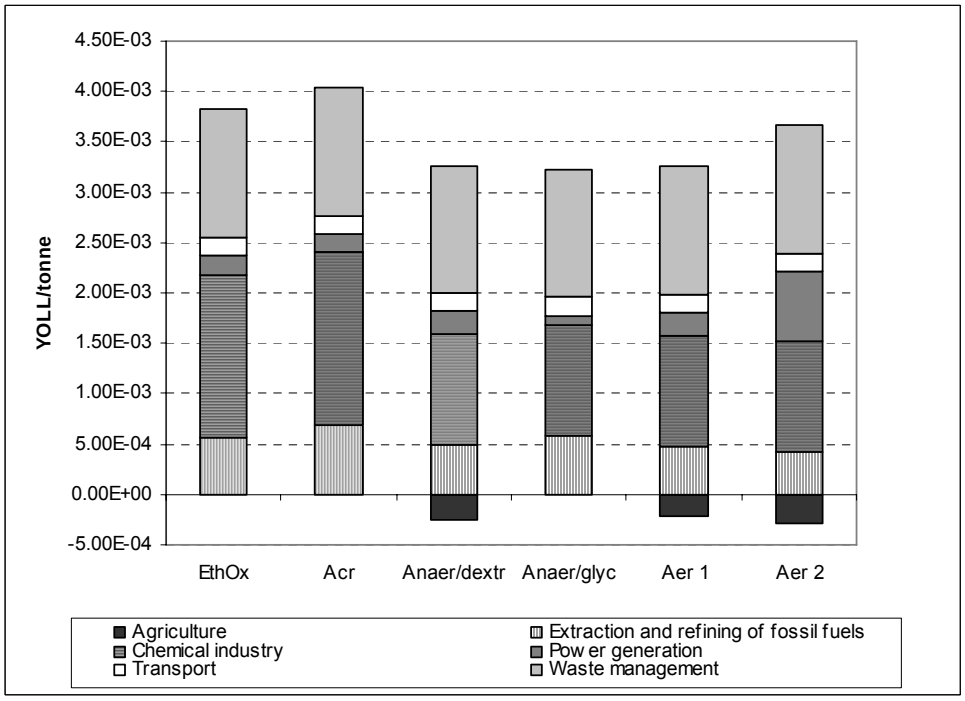


Figure 5-2: Results for PTT showing relative contributions of the different sectors (for abbreviations on the x-axis see second column in Table 5-5)

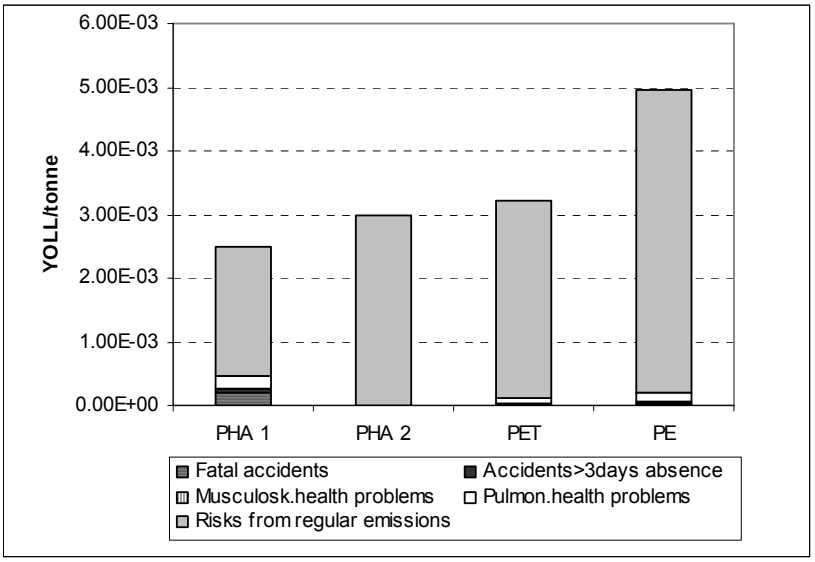
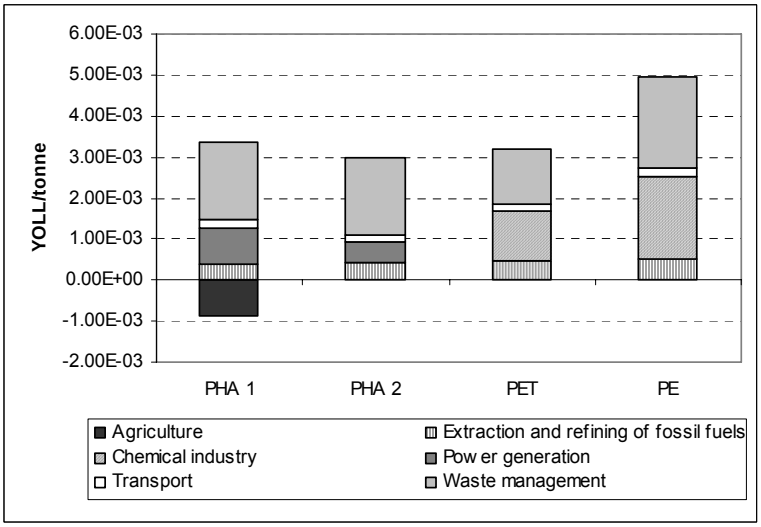


Figure 5-3: Results for PHA, PET and PE showing relative contributions of the different factors (for abbreviations on the x-axis see second column in Table 5-5)



Notes:
- Values for chemical industry include equivalents of power generation.
- Glycerol is considered as “waste product” (of biodiesel production. For this reason no impacts related to agriculture are allocated to glycerol.

Figure 5-4: Results for PHA, PET and PE showing relative contributions of the different sectors (for abbreviations on the x-axis see second column in Table 5-5)

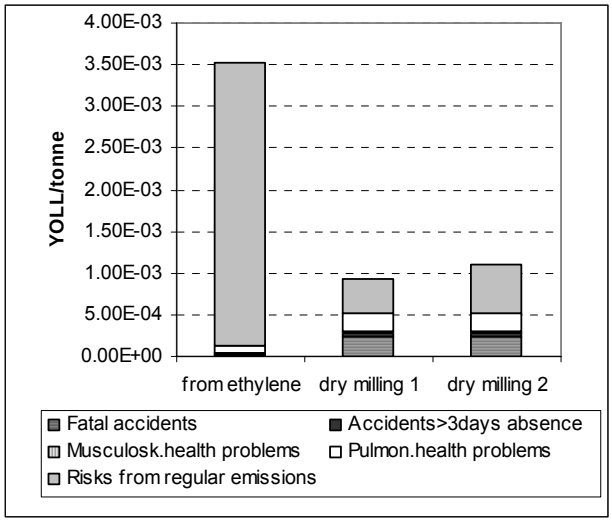


Figure 5-5: Results for ethanol showing relative contributions of the different factors (for abbreviations on the x-axis see second column in Table 5-5)

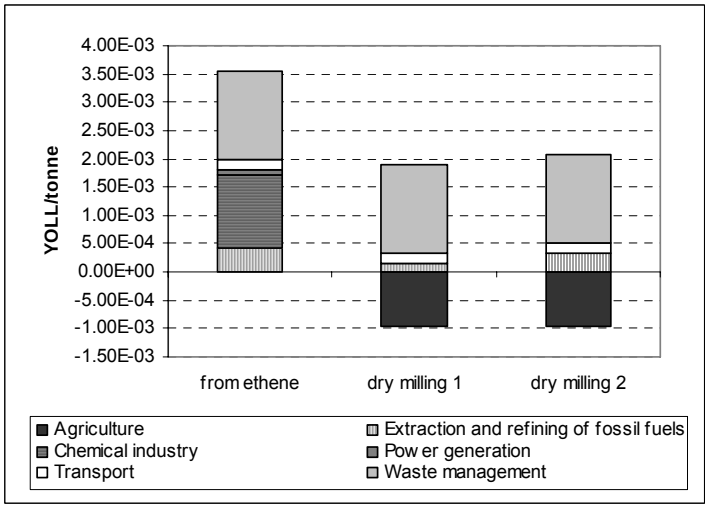


Figure 5-6: Results for ethanol showing relative contributions of the different sectors (for abbreviations on the x-axis see second column in Table 5-5)

5.1.3 Uncertainty analysis

To assess the quality of the results we conducted an uncertainty analysis, which comprises the following elements:

- Ranges of input data are determined (only for accidents).
- Coverage of emissions in SimaPro impact assessment is determined (not all emissions are defined by the EPS 2000 method).
- Impact assessment of emissions using EPS 2000 method is compared with an impact assessment using CML baseline 2000 and Ecoindicator 99.
- Plausibility of results is checked by comparison with values taken from other literature sources
- Uncertainties of assumptions are determined.

Ranges of input data

The data sources found report different values on accidents. The ranges are shown in Table 5-6.

	Fatal accidents		Accidents > 3days absence	
	Arithmetic mean	Range (around arithmetic mean value)	Arithmetic mean	Range (around arithmetic mean value)
Agriculture	1.47E-4 #/TJ	± 3%	0.0777 #/TJ	± 3%
Extraction and refining of fossil fuels	2.36E-7 #/TJ	± 25%	No range	± 0%
Chemical industry	1.65 E-5 #/TJ	± 28%	No range	± 0%
Power generation	3.61E-6 #/TJ_e	± 1%	0.00137 #/TJ	± 10%
Transport	3.19E-10 #/tkm	± 31%	1.99E-7 #/TJ	± 44%

Table 5-6: Data ranges for fatal accidents and accidents with >3 days absence

Uncertainty analysis for accidents and illnesses

To convert the number of occurences of accidents and health problems to "years of lost life" assumptions are made concerning the time period in which a person suffers. This uncertainty analysis addresses this time period because it can be crucial for the results.

- For fatal accidents it is assumed that an accident reduces a life on average by 34.75 years. It is assumed that an average employee is 42.5 years old based on a working age of between 20 and 65. The real age might be lower because people might start working before the age of twenty and due to illness or death the group of employees older than 42.5 might be smaller. Therefore the uncertainty range for the age of an employee struck by a fatal accident is assumed to be ± 10 years. This brings the uncertainty range of the risk to ± 29%
- For accidents with >3 days absence from work the average period of absence is assumed to be 30 days. If an uncertainty of 10 days is assumed the uncertainty in the risk is ± 33%.
- For pulmonary health problems the assumptions are very rough. 10 years at max of suffering morbidity is assumed. If this period shortened with five years or extended to the period a person looses life due to a fatal accident (34.75 year) the uncertainty is roughly -50% / + 150%.
- For muscoskeletal health problems 10 days of absence are assumed for 1 muscoskeletal health problem. An uncertainty of 5 days could be assumed which gives a risk uncertainty of ± 50%.

For the case "Ethanol-dry milling 1" the contribution of the regular emissions to the total risk is lowest (and thus the contribution of factors which we just discussed is highest). When the uncertainties identified above are applied to this case the lower risk value is 0.00073 YOLL/tonne and the upper risk value is 0.001369 YOLL/tonne (original value was 0.000934 YOLL/tonne). This means that the maximum uncertainty of the results for all cases is -22% and + 47%. In conclusion, the uncertainty range for accidents and illnesses is rather limited and the final result for the total risk remains within the same order of magnitude (only for ethanol the risk pattern changes somewhat while for all other cases emissions remain the dominant risk source).

Coverage of emissions by EPS 2000

For each of the six sectors included in this risk assessment emissions impacts are determined using the EPS 2000 method in SimaPro 6 (PRé Consultants 2004). However, only a relatively small share of the emissions for which data were found are defined in this method (11-32%, see Table 5-7). For all other types of emissions no impact results are calculated. This means

that the impacts determined with the EPS method represent an underestimation of the real impacts.

Sector	Impacts based on:	Fraction of emissions defined in EPS 2000 *)
Agriculture	Grain maize IP, at farm/ CH S	11%
Extraction and refining of fossil fuels	EU-15 emissions "mineral oil and gas refineries"	32%
Chemical industry	EU-15 emissions "basic organic chemicals"	28%
Power generation	CENTREL/NORDEL/UCTE medium voltage electricity mix, at grid	11%
Transport	Transport, lorry 32 t/RER S	11%
Waste management	Disposal, polyethylene terephtalate, 0.2% water, to municipal incineration/ CH S	11%

*) This is calculated as the number of substances that are defined by EPS 2000 divided by the number of substances for which emissions data are available. It is NOT based on absolute amounts of emissions. For agriculture, power generation, transport and waste management the coverage is 63 out of 552 substances. For extraction and refining of fossil fuels the coverage is 16 out of 50 substances and for chemical industry the coverage is 16 out of 57 substances.

Table 5-7: Coverage of emissions by EPS 2000

Comparison EPS 2000 impact results with CML 2 baseline 2000 and Ecoindicator 99

The emission impacts reported in this chapter have been calculated with the EPS 2000 method. To assess the quality of the results calculated with EPS 2000 the results were recalculated with two other widely known methods, i.e., CML 2 baseline 2000 and Ecoindicator 99. The comparison across the methods is, however, difficult because each of them uses a different unit to express the impact; CML 2 baseline 2000 expresses damage to human health in "1,4-dichlorobenzene equivalents (1,4-DB-eq)" and Ecoindicator 99 uses "disability adjusted life years (DALYs)" as common metric. For comparison, it is therefore necessary to know the conversion factor between 1 kg 1,4 dichlorobenzene equivalents and 1 YOLL and likewise between 1 DALY and 1 YOLL. These conversion factors were approximated as follows:

A given impact expressed in 1,4-DB-eq could, theoretically, be translated to YOLL by importing the 1,4-DB-eq quantity as an emission to air in the EPS 2000 method and calculating the impact in YOLL. The problem is, however, that 1,4-dichlorobenzene is not included in the EPS 2000 method. Therefore a substance was selected with similar properties as 1,4-dichlorobenzene. Ideally this would be another halogenated aromatic. Since no such compound is defined in EPS 2000, ethylbenzene was chosen. The toxicity of ethylbenzene as an emission to air is 0.97 kg 1,4 DB eq/ kg.

When recalculating all impacts with CML 2 baseline 2000 and importing the results in kg 1,4-DB-eq as kg ethylbenzene in EPS 2000, results in YOLL were obtained that ranged from a factor 0.62 to 13.3 compared to the original results.[102] While this range is large, it still seems acceptable in view of the large number of assumptions and the uncertainty and incompleteness of the input data used.

[102] YOLL(based on ethylbenzene)/YOLL(original) is as follows:
- Mineral oil and gas refineries: 1.16
- Basic organic chemicals: 0.62
- UCTE electricity: 3.48
- CENTREL electricity: 3.92
- NORDEL electricity: 3.45
- PET incineration: 13.3
- Lorry 32 t: 4.9
- For agriculture (maize) results cannot be compared for EPS 2000 gives negative result and CML 2 baseline 2000 gives positive result.

To compare the results obtained with EPS 2000 with results obtained with Ecoindicator 99 the impacts of several compounds included both in EPS 2000 and in Ecoindicator 99 were compared by determining the ratio. The results were found not to be consistent.[103] It was therefore concluded that it is not possible to compare results of the two methods EPS 2000 and Ecoindicator 99.

Plausibility check by comparison with other literature data
The results for PTT, PHA, PET and PE, expressed in YOLL, have been checked for plausibility by relating them to gross impacts of all sectors in Europe and by comparing the plastic industry's energy consumption relative to the total primary energy supply (TPES) in Europe.
In Europe, the current average production of plastic per capita is 145 kg plastics per person (55 Mtonne plastics produced p.a. divided by 380 million inhabitants). Plastics are produced by the chemical industry. Using energy data published by the IEA (2002) the primary energy consumption by the chemical and petrochemical industry can be estimated (149 Mtoe). Total primary energy supply (TPES) in 2000 was 1461.91 Mtoe. This means that, in Europe, primary energy use by the chemical and petrochemical industry was 10% of total TPES.
145 kg plastics per capita can be translated to YOLL by taking the results from this research. Assuming that all plastics consist of either PTT, PHA , PET or PE, the average risk of 145 kg plastics per capita is 0.5 YOLL/1000 persons. The total impacts of all emissions of all sectors in Europe in 2001 has been estimated by Brand et al. (2004) to amount to 6.24 YOLL/1000 persons. The share of the plastics then is 0.5/6.24, which gives 8%. This is consistent to the 10% derived above (estimate based on energy use).

Uncertainties of assumptions
The method described above contains numerous assumptions and estimates. This results in a considerable level of uncertainty of the final results:

- The choice of reference units and the translation to process inputs is based on a generic approach. It therefore contains uncertainty. For example, it was assumed that 1 TJ total crop output from agriculture can be translated to all bio-based feedstocks, that crude oil consumption in case of "extraction and refining of fossil fuels" covers all primary energy used and that fossil feedstock consumption is a good estimate for all petrochemical feedstocks in case of "chemical industry".
- Data taken from the energy balance of OECD countries are from the year 2000. Therefore these data might be outdated.
- Data on the total amount of road and rail freight transport are from the year 1999. They might be outdated.
- It is assumed that all categories from the EPS 2000 method (e.g., morbidity and nuisance, see Table 5.3) can be translated to YOLL by normalizing according to the weighting factors.
- The conversion of accidents to YOLL is based on very rough estimates. The same holds for the conversion of health problems to YOLL.
- For the conversion of emissions to YOLL a generic approach is used for the sectors "extraction and refining of fossil fuels" and "chemical industry". The approach of taking

[103] Some examples (EPS 2000 ↔ Ecoindicator 99 in YOLL/ DALY):
- Ammonia: 0.45
- Benzene: 13.5
- Formaldehyde: 33.24
- PAH: 4396

total emissions of each sector and dividing them by respectively the total crude oil consumption and the total fossil feedstock consumption is based on estimates and using these outcomes in final calculations is therefore subject to uncertainties.

- The use of SimaPro 6 (PRé Consultants 2004) for calculations of environmental impacts contains uncertainties because not all substances are defined by the EPS 2000 method. Therefore the calculated impacts are underestimated and they represent only an indication of *real* impacts.
- For calculations concerning electricity, "medium voltage electricity" is assumed. It is not clear whether this is the same type of electricity used in the production of PTT, PHA and ethanol.
- The calculations for transport are based on the assumption that all transport takes place with a 32 tonne load-capacity lorry over 500 km.
- Calculations for waste incineration are based on PET and it is assumed that impacts for 1 TJ of PET can be applied to 1 TJ of other plastics (PTT and PHA) and ethanol as well. This is a rough approximation.
- Process energy and feedstock energy needed to produce petrochemicals is based on estimates.
- Data on accidents and illnesses from EC (2002) and EC (2004) are based on slightly different categories than the categories used in this research. For example, this research uses the category "extraction and refining of fossil fuels", whereas the data on accidents are based on the category "manufacture of coke, refined petroleum products and nuclear fuel".

5.1.4 Conclusions

In this chapter a method for generic risk assessment has been successfully developed and applied. The method covers the total process chain for petrochemical and bio-based products from cradle to grave. This chapter focuses on conventional risks to human health, thereby taking into account accidents, illnesses and external risks imposed on the public due to emissions and technological disasters. Risks related to genetically modified (GM) micro-organisms and crop plants are excluded.

By far the most important source of risks (expressed in terms of Years of Lost Life, YOLL) are external risks caused by the release of emissions from regular operation, followed by pulmonary health problems of workforce and accidents of workers (fatal accidents and accidents with more than three days of absence). External risks imposed on the public due to technological disasters are found to be negligible.

According to the results the conventional risks related to all bio-based products studied are lower than for the petrochemical products. While these average results are in favour of bio-based production the uncertainties involved in the assessment are large to very large. Taking into account the uncertainties caused by the ranges of input data, the (incomplete) coverage of the emissions by EPS 2000 and the uncertainties of the assumptions made in this study the differences in the results between bio-based and petrochemical products (although in favor of bio-based production) definitely fall into the uncertainty range. **Therefore, in view of the considerable uncertainties involved, application of our method leads to the conclusion that the conventional risks of biotechnologically produced chemicals (risks related to**

genetically modified micro-organisms and crop plants excluded) are comparable to those of chemicals derived from fossil fuels.

This finding is partly determined by the methodology which i) yields results that are largely driven by energy use (determines emissions from regular operation) and ii) makes use of generic risk factors for chemical industry. The latter is justified because the type of raw materials and the type processes do not differ essentially from each other. **However, if White Biotechnology materializes, new raw materials, intermediates and final products will be handled. This inevitably leads to new risks which will need to be identified and mastered. As experienced in the petrochemical industry in the past, industrial accidents will also happen in the emerging bio-based sector. There is, however, no reason to assume that the risks in the emerging bio-based sector cannot be mastered. To minimize the frequency and the hazard of incidents a suitable safety code needs to be developed for the White Biotechnology industry.**

5.2 Risks related to GMO

Biotechnology has the potential to play an important role in bulk chemical production in the future. Drivers for the application of biotechnology in chemical processes (compare Chapter 3 and 4) are the lower use of non-renewable energy, the lower greenhouse gas emissions, economic advantages (if the required technological progress is made) and new products with superior functionality. However, biotechnological production is relatively new and not fully accepted by the public. For example, production with genetically modified organisms (GMOs) requires special emphasis on possible risks related with their use. Most importantly, the public is concerned about unknown or unexpected side effects associated with the use of GMOs in natural environments or agricultural products meant for food production. Therefore, the risk of hazards must be thoroughly evaluated prior to application of new GMO constructs. This is a demanding task because a general assessment covering all GMOs is not possible; each construct has its specific characteristics and may have different effects on nature or human health. Therefore, each newly developed construct needs to be evaluated individually on proposed effects with regard to the products made from the construct and the neighbourhood of production facilities where GMO constructs are used.

Biotechnological production involves living organisms like bacteria, yeasts or plants, or products derived from living organisms, like enzymes. Special features in certain species are important for industry, for instance PHA production in the bacterium *Ralstonia eutropha*. Although interesting for industry, the prime function of these features is species survival in nature which are maintained under strong environmental selective pressure. PHA, for example, is a storage compound which plays an important role as energy source for *R. eutropha* under nutrient limiting conditions. Metabolic pathways for the production of compounds in living cells require specific sets of enzymes. Like all proteins, enzymes are polymer strands made of amino acids, arranged in specific order and often folded in complex structures. The amino acid order in protein strands are encoded by DNA arranged in chromosomes in the cellular nucleus of eukaryotes, like fungi, plants and animals, or in single chromosomes in prokaryotes (organisms which do not possess nuclei in their cells) like bacteria. All cellular processes are transcribed from DNA, in chromosomes or outside chromosomes on plasmids (extra chromosomal DNA) or in plastids (subcellular organelles). These three components comprise the cell's total inheritable information present, which is called the "genome". DNA is a polymer strand composed of four different nucleotides arranged in specific order. Codons[104] consisting of three nucleotides in DNA strands is encoded into one aminoacid in protein strands. All codons in a DNA strand, coding for one protein strand is called a "gene". Proteins are, however, not directly transcribed from DNA, but via RNA acting as intermediate molecules.

Prior to cell division, DNA in chromosomes must be exactly reproduced in order to subdivide all inheritable information to both daughter cells. However, during DNA reproduction, mistakes (mutations) may occur, leading to variations in genomic composition. Most commonly mutations are detrimental or even lethal and only rarely mutations act beneficial to organism survival in nature. Therefore, natural variation and environmental selection are the driving forces behind evolution. Genomic variation is important for adaptation under shifting

[104] A codon represents an information code that stands for a specific amino acid.

environmental conditions. Genomes of species are composed of different genes and among individuals of the same species considerable genomic variation may exist. Genomic rearrangements by sexual reproduction require separation of chromosomes into reproductive cells (gametes), like egg cells, pollen in plants and sperm in animals and fusion of gametes will result in new genetic combinations. After sexual reproduction, chromosomes in cell nuclei of progeny (offspring) will be rearranged and extra chromosomal DNA present in cell organelles directly originate from the female parent (maternal DNA transfer). Mitochondria are important for cellular energy production, whereas in plastids photosynthesis takes place. Both cell organelles have separate chromosomes independently functioning from chromosomes present in nuclei. In prokaryotes (e.g., bacteria or algae), however, sexual exchange of DNA comparable to eukaryotic species (e.g. plant cells), does not exist. DNA exchange between bacteria may occur via three processes: transformation, conjugation and transduction. Transformation requires DNA uptake from the environment and incorporation into the genome. DNA may be released from dying cells and may persist in the environment unprotected as "naked" DNA or in protected form, e.g. encapsulated by clay minerals (Davison 1999). Conjugation requires extra chromosomal DNA, arranged in plasmids, which is transferred via living cell contact. Plasmid transfer requires special functions encoded by genes on plasmids which are important for transfer; so called mobilization (*mob*) and transfer (*tra*) genes. For transduction, DNA is exchanged between different bacteria via bacteriophages (cell-less bacterial parasites, comparable with viruses in eukaryotes).

Breeding requires genomic rearrangements by crossing which yields varieties that are beneficial for mankind. New varieties are selected and tested by man using breeding programs with genotypically different parents. These varieties are selected only for a few traits, whereas numerous other unknown genomic rearrangements concomitantly may occur during crossing. Breeding programs and subsequent tests on expected traits are comprehensive and laborious. During crossing, borders between eukaryotic species cannot easily be passed, although interspecies DNA exchange between prokaryotes exists. Genetic modification in breeding programs requires molecular isolation of genes from a donor variety or strain and incorporation into the genome of a recipient variety or strain (host), using modern molecular biological tools. Genetic modification differs from conventional breeding in the sense that only selected genes (transgenes or heterologous DNA) are transferred, most commonly passing interspecies barriers (crossing also the bonds beyond totally unrelated species, e.g., between bacteria and plants). Varieties or strains resulting from genetic modifications, respectively called genetically modified (GM) plants or micro-organisms, carry transgenic constructs in their genomes (in chromosomes or in extra chromosomal elements like plastids or plasmids). The precise location of the transgenic construct within the genome (insertion site) is not always well defined and sometimes additional DNA, like antibiotic marker genes, are incorporated. Eventual effects from genetically modified constructs can be explained from characteristics of the heterologous construct (transgenic construct, recombinant construct) and the host (organism carrying recombinant DNA, e.g., bacteria or plants) separately, although new and unexpected traits may result from combined effects of transgenic construct and host (Hilbeck 2001). Therefore careful risk assessment of new transgenic constructs will be required with respect to safety and human health prior to application in bulk chemical production.

5.2.1 Risk assessment approach for genetically modified organisms

Accidental or deliberate releases may result from applications with GM micro-organisms and plants in bulk chemical production. Although GM micro-organisms will be applied under contained conditions, i.e. physically, chemically and sometimes biologically separated from the environment, these strains may be released after accidents, e.g. by failure of equipment or leakages (Figure 5-7). GM plants, on the contrary, will be planted into open fields and unlimited spread of pollen and seeds by wind, water and animals to adjacent fields or to nature (Figure 5-7) will continuously occur. Also, volunteer plants (plants which survived from previous harvests, e.g. as tuber or seed) may appear in the same field in succeeding crops resulting from outgrowth of remaining plants or plant organs like tubers. Spread from open fields will therefore be the consequence of the application of GM plants for purposes of bulk chemical production.

Transmission of GMOs from the production area, either after accidental releases of GM micro-organisms or by spread of GM plants, may result in contamination of nature or consumable products for humans or animals. Contamination does not necessarily imply hazard. Potential hazards may be ecological disturbances or contamination of food eventually resulting in food poisoning. Risk assessment of GMOs focuses on impact analysis, i.e. occurrence of hazardous effects after releases. Severity of impact after GMO release will differ for each GMO construct applied and impacts lowest in ranking of severity are those that do not pose any effect on nature or human health. Impacts after GMO releases suspected to be harmful, either for the environment or for human health, are higher in ranking whereas the severest cases will be impacts after release of GMOs which clearly demonstrated to be threatening to nature or human health. Not only the nature, but also the quantity of transmitted GMOs must be considered in impact analysis. Volumes of material containing GM micro-organisms accidentally released from production plants may be considerable, but most accidental releases will nevertheless only cause local contaminations. Release of GM plant materials from production fields may be relatively small but constant in time and contamination may cover larger areas. Risk must therefore be calculated from each individual incident concerning GMO releases by multiplying the hazard with the probability of exposure to nature or food sources in agriculture.

Risks for nature are ecological disturbances like invasion and blooming of released GMOs in ecosystems, resulting in extinction of species. GMO contaminations may directly interfere with natural populations e.g. by production of toxins or indirectly by competition for nutrients, water, light and other important factors essential for survival of other species. Interference with ecosystem functioning like nutrient cycling is an important risk. However, due to the complexity in functioning of ecosystems, effects may be unpredictable. Novel GMOs may be extensively tested for direct effects under laboratory or greenhouse conditions but other, unexpected, effects may reveal upon release into nature. On the other hand, particular functions in ecosystems are redundant and the function of affected populations can easily be restored by other populations. Natural fluctuations in ecosystem composition may be considerable, e.g. due to weather or seasonal effects. In order to make statements about effects caused by GMOs on natural ecosystems, baseline fluctuations must be understood (Wolfenbarger and Phifer 2000). This information is often not available thus limiting precise predictions of GMO impacts on nature.

Risks for animal or human food chains are food contamination caused by released GMOs. Products from the host or expressed products from the recombinant gene may also cause food poisoning. Food poisoning may result from production of toxins or allergens causing direct

effects on consumers or may result in accumulation of toxins or allergens in tissues of primary consumers resulting in toxic or allergenic effects on consumers at the end of the food chain, mostly humans. Human and animal health is a major concern for the application of novel GMO constructs and therefore direct effects must be tested extensively prior to marketing. However, effects may become less predictable when recombinant DNA is transmitted to other species in nature (Davison 1999). For example, antibiotic resistance genes, commonly present in recombinant DNA constructs (transgenic constructs), may be transmitted to pathogenic micro-organisms resulting in antibiotic resistant pathogens. These concerns can easily be eliminated by exclusion of antibiotic resistance genes in GMO constructs by making use of marker-free constructs. Another strategy to eliminate potential risks related to GMOs is to restrict survival or sexual exchange of recombinant DNA upon release. Micro-organisms can be restricted in survival by inactivation of genes important for survival under ambient conditions in natural ecosystems, like genes important for production of essential nutrients. Occasionally micro-organisms are already limited in their survival under specific conditions, like the gut bacterium *Escherichia coli* which poorly survives in soil ecosystems. Plants can be restricted in sexual exchange of recombinant DNA by integration into extra chromosomal DNA present in plastids. In contrast to DNA present in chromosomes, extra chromosomal DNA is not integrated into pollen and crossings will not result in transgenic hybrids.

Having provided insight into the principles of the transfer of genetic information and the risks involved, we will now discuss separately White Biotechnology (Section 5.2.3) and Green Biotechnology (Section 5.2.4).

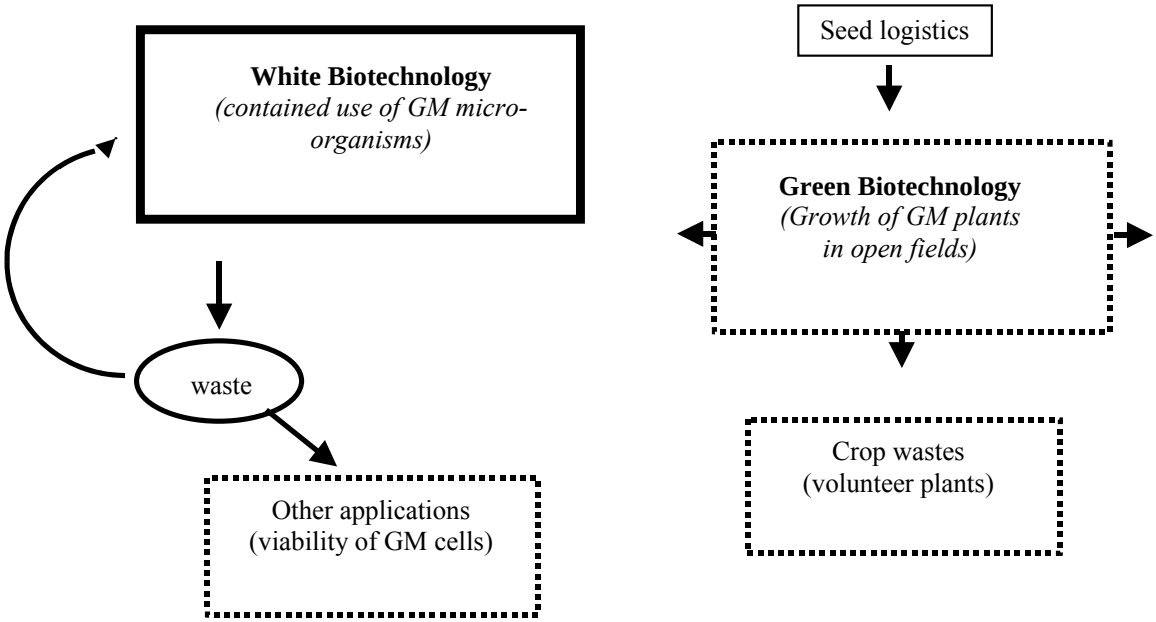


Figure 5-7: Difference in containment of GM micro-organisms and plants, respectively used in White and Green biotechnology (GM micro-organisms are applied under contained conditions, whereas GM plants will be grown in open fields)

5.2.2 Use of GMOs in White Biotechnology

White Biotechnology is the production of chemicals and fuels by application of fermentation and enzymatic processes. Genetically modified micro-organisms *may* be used in fermentation processes and for the production of the enzymes. Production by means of White Biotechnology takes place in reactor vessels and is thus contained, i.e. physically separated from the environment. The large-scale application of White Biotechnology not only leads to increased risks of accidents, but also to large amounts of waste materials possibly containing living cells or materials derived from these cells like transgenic DNA (Doblhoff-Dier et al. 2000). Industry will therefore be confronted with possibly costly procedures to prevent accidental discharges of GM micro-organisms from production facilities and total eradication of living GM cells from waste products (in the Generic Approach discussed in Chapter 3 it is assumed that biomass waste is incinerated with energy recovery). It is, however, questionable whether *all* releases of GM micro-organisms, either by accident or via waste, will result in unacceptable risks for nature and, or human and animal health.

Accidental discharges of GM micro-organisms from production facilities may be the result of constant (unattended) leakages or suddenly under force, e.g. caused by higher pressure. The nature of the accident will have consequences on the extension of the contaminated area and on the amount of released GM micro-organisms. In case of accidental discharges it is expected that contamination will remain local and most commonly contamination will be restricted to industrial areas (Noordover et al. 2002). Decontamination of the accident site may be done with chemical, biological or physical methods aimed to eradicate the vast majority of GM micro-organisms although total eradication can not always be guaranteed. Deliberate releases of GM micro-organisms from production facilities may be the result of disposal of wastes still containing living GM micro-organisms or by application of products derived from these reactor wastes, e.g. for commercial purposes like agriculture (Andersen et al. 2001; Doblhoff-Dier et al. 2000). The consequences of disposal or re-usage of reactor waste materials contaminated with GM micro-organisms would be spread over extensive areas and possibly contaminated areas may remain unidentifiable. It is therefore of utmost importance that disposed wastes or materials processed from reactor wastes are free of GM micro-organisms which are suspected to be threatening to nature or human health. For these GM micro-organisms, total eradication of living cells from reactor wastes prior to disposal or further processing is required. However, for non-threatening GM micro-organisms total eradication may become a useless endeavour especially considering the enormous quantities required to be sterilized. After thorough sterilization of reactor wastes questions still remain like: are the methods applied to screen for GM micro-organisms, which may have survived the sterilization process, sufficiently reliable to detect all living cells, or what will happen with products released from dead GM micro-organisms like transgenic DNA? A new question thus arises; to what extent are deliberate releases of GM micro-organisms still acceptable?

Living cells of GM micro-organisms released into natural environments like soils, water, plants, animal gut and other ecosystems will survive for short or more extended periods in time, depending on ambient conditions and physiology of the host cell (Van Elsas et al. 1990; Dighton et al. 1997; Van Veen et al. 1997; van Overbeek and van Elsas 2001; Noordover et al. 2002;). It is expected that GM bacteria may even be more reduced in their survival than their unmodified relatives due to the extra metabolic load caused by heterologous gene expression (De Leij et al. 1998). Like all biological agents, GM micro-organisms may

reproduce in nature, thus possibly extending the contaminated area. Also products released from living or decaying dead cells of GM micro-organisms like transgenic proteins and poly nucleic acids may pose effects on nature or human and animal health. Different methods can be applied to construct GM micro-organisms aimed to reduce threat or restrict survival outside production facilities. Extra genetic modifications may be inserted in GM micro-organisms which kill cells after discharges from production facilities (Knudsen et al. 1995). However, mutations in transgenic constructs or transfer of transgenic DNA to other species may lead to new transgenic combinations which demonstrate improved survival upon releases into nature. Gene transfer incidences take place in natural environments, which must be concluded from the genomic structure present in bacterial species whose genome has entirely been sequenced, although the frequencies of these incidences must be considered as extremely low (Davison 1999). Occurrence of new transgenic combinations in nature does not directly imply improved survival or higher risks. In almost all cases, mutations will lead to weaker instead of improved adaptations under ambient circumstances. Even in those rare cases where better adapted transgenic combinations may appear, the appropriate selective forces are still required to favour further outgrowth and colonization (Nielsen et al. 1998). Products derived from GM micro-organisms like transgenic DNA, RNA and proteins will be broken down to their elementary building blocks, nucleotides and amino acids, by micro-organisms residing in natural ecosystems. Only DNA polymers can be taken up and incorporated into genomes of micro-organisms residing in natural ecosystems. The lifetime of large DNA polymers released from dead cells is extended by binding to clay particles in soils (Davison 1999). However, in studies performed in agricultural field soil mixed with fertilizer made from fermentation waste material, transgenic DNA could not be detected with sensitive molecular techniques (Andersen et al. 2001). On the other hand, in the same study DNA was demonstrated in the fertilizer before mixing to soil indicating that DNA must have been degraded soon after application to soil. Eventual transformation incidences from transgenic DNA bound to clay particles are also expected to be very low (Davison 1999). Again new transgenic combinations need to result in better adaptation to ambient conditions and the appropriate selective forces must be present to favour further outgrowth and colonization (Davison 1999; Nielsen et al. 1998).

It can therefore be concluded that GM micro-organisms used in White Biotechnology, and not posing a rational threat by the nature of the transgenic combination to nature or human health, can safely be released into other environments. Secondary, unexpected, effects related to mutations or transfers of transgenic DNA to other species are expected to occur only at extremely low frequencies, if occurring at all. The occurrence of secondary effects upon releases of GM micro-organisms into other environments can be lowered by making use of transgenic constructs in self-contained host organisms. Absence of any secondary effect can never be absolutely guaranteed due to complexity and limited knowledge on functioning of natural ecosystems.

5.2.3 Use of GM plants in green biotechnology

Green biotechnology comprehends production of bulk chemicals in agricultural crops. Production of chemicals in GM plants will be novel for industrial application and requires growth in open systems like agricultural fields. The main advantage for the use of GM plants

in bulk chemical production is the potential to produce large quantities at a relatively low cost.

Production in open systems implies that there is no physical separation from the neighbouring environments so that there is in principle no restriction to transmission of GM DNA in pollen and seeds (e.g. Chen et al. 2004). In Wolfenbarger and Phifer (2000) two main pathways for spread of transgenic DNA are described upon introduction of GM plants into open fields. The following steps are discriminated in pathway I: "1) survival outside of cultivation, 2) reproduction outside of cultivation, 3) self sustaining populations", and in pathway II: "A) pollen flow to wild relatives, B) hybrid formation, C) hybrid survival, D) hybrid reproduction and E) introgression of genes into wild species". Both pathways ultimately may lead to spread and persistence in nature resulting in economic and environmental harm. Case studies on field releases with different GM plant constructs, discussed in Wolfenbarger and Phifer (2000), made clear that the occurrence of at least some of the proposed steps must be regarded as realistic.

The occurrence of economic and environmental harm upon GM plant field releases depends on the GM constructs and the measures applied to control spread of pollen and seeds from the location of cultivation. Effects of GM constructs on non-target populations were investigated for Bt (*Bacillus thuringiensis* toxin) crops on arthropods (Hilbeck 2001; Sisterson et al. 2004; Candolfi et al. 2004), cysteine proteinase inhibitor potato plants on aphids (Cowgill et al. 2004) and T4 lysozym potato plants on plant-associated communities (Heuer et al. 1999; Van Overbeek et al. 2005). These studies did not reveal any observable effects caused by applied transgenic crops in open fields. Other proposed effects may be transfer of transgenic DNA, especially antibiotic resistance markers, to plant-associated communities. DNA of GM plants appeared to resist for several months in soil (Paget et al. 1998; Ceccherini et al. 2003). Transformation of *Acinetobacter* sp. strain BD413 has been demonstrated in vitro using transgenic plant DNA containing kanamycin resistance marker gene *npt*II (Nielsen et al. 2000) and its ability for transformation was demonstrated in tomato plants (Kay et al. 2001). However, DNA transfer from GM plants has never been experimentally demonstrated. If occurring at all, certain measures proposed to restrict gene transfer from plants to plant-associated bacteria have been proposed by Kay et al. (2002), which are: genetic modifications in plastids and not in chromosomes and absence of DNA sequences homologous to highly transformable species like *Acinetobacter* spp. in transgenic constructs. Whether DNA transfer will result in more antibiotic resistant populations in nature is also questionable, especially when realizing that natural ecosystems like soils must be considered as sources instead of sinks of antibiotic resistance genes (Van Overbeek et al. 2002; Heuer et al 2002).

Nowadays marker-free constructs are available (Ebinuma et al. 1997; Lamtham and Day 2000) and it is expected that these constructs will replace constructs with antibiotic resistance markers in the near future. Spread of transgenic DNA from GM plants to unmodified crops is possible (Ma et al. 2004; Gruber et al. 2004) and may result in economic harm. Crossing or contamination with GM plants will result in contamination of non-modified crops. In other agriculture systems, like organic farming systems, these contaminations are unacceptable and organic farmers confronted with high levels of GM contamination in their crops can not meet their required standard for production. Contamination of non-GM plants with transgenic DNA can be controlled, e.g. by logistic separation of GM seeds from non-GM seeds, although this has not been proven to be a reliable approach so far, and prevention of sexual exchange of transgenic DNA by using extra chromosomal (e.g. in plastids) instead of chromosomal insertions. Further, spatial separation of GM crops from organically farmed crops will minimize contamination by gene flow from pollen and seeds.

It must be concluded that technological and agronomical measures can control environmental and economic effects associated with the growth of GM plants in open fields. Absence of any noticed effect caused by growth of transgenic plants does not indicate total absence of any effect. So far most studies done with GM plants were carried out in small-scale field trials for maximally two or a few consecutive years. Unexpected effects may result from scale enlargement by commercial growth of GM plants in vast production areas over longer periods in time, as proposed for production in Green Biotechnology. However, world-wide production with many different GM crops is still increasing and new information may soon become available from commercial experiences.

5.2.4 Genetically-modified PHA-producing micro-organisms and plants

Plastics represent a large share of the output of current bulk organic industry and bio-based plastics would be among the key products if biotechnology becomes widely used in chemical industry. Bulk quantities of bio-based plastics can be produced either by means of GM micro-organisms in production reactors (White Biotechnology) or in GM plants on open fields (Green Biotechnology). Polyhydroxyalkanoates (PHA) like polyhydroxybutyrate (PHB) and polyhydroxyvalerates (PHV) represent an example for a compound which can be produced both by White Biotechnology and Green Biotechnology. In nature these compounds serve for energy storage in bacterial cells (Kimura et al. 2003). It has been demonstrated that PHAs are degraded by hydrolase-like enzymes from different *Pseudomonas* species present in nature (Colak and Güner 2004). These and possibly other processes make materials made from PHAs biodegradable. Biodegradability can, for example, be an asset for packaging or for medical applications (Zinn et al. 2001). Different GM constructs have already been made in different hosts like bacteria, yeast and plants (Table 5-8). Constructs described in literature will be discussed here with special emphasis on effects on nature and humans.

PHA-producing transgenic constructs have been made in bacteria, *R. eutropha* and *Aeromonas hydrophila,* and yeast, *Arxula adeninivorans,* using genes originating from the PHA pathway in *R. eutopha* (*pha*) or a precursor gene in this pathway (*yaf*H). Also GM plants have been constructed using genes derived from prokaryotic PHA pathways (via bacteria). Flax and tobacco were used for construction of PHA-producing transgenic plants by insertion of *phb* genes from *R. eutropha*. PHA-producing plant cells were also constructed from potato by insertion of the *pha* gene from *P. oleovorans*.

It is unlikely that all constructs will be applied for commercial production of bio-based plastics. Suspensions of plant cells, for example, are hard to maintain in reactors and will produce too low quantities of PHA. Bacteria or yeast equipped with *pha* genes are more realistic for commercial applications. However, the constructs summarized in Table 5-8 carry their heterologous genes on plasmids which still possess genes required for conjugation. Presence of *pha* genes on plasmids may still be preferred because of their higher copy number (number of plasmids in the host) in cells. Antibiotic resistance markers on plasmids may be transferred to other species contributing to increased antibiotic resistances especially in human pathogens present in clinical environments. However, the genes used confer resistance to kanamycin, streptomycin and ampicillin which are antibiotics that are rarely used for therapeutic treatments against bacterial diseases in humans. Flax and tobacco plants equipped

with *pha* genes are also realistic for commercial application, although both constructs still carry antibiotic resistance markers. The heterologous gene is located in plastids which exclude sexual exchange of transgenic DNA to non-modified plants after pollen release. Both plants are not used for production of food for humans or domestic animals which make contamination of human or domestic animal food chains unlikely. However, PHA from transgenic tobacco plants may still be consumed via smoking after contamination of non-modified tobacco plants grown with the purpose of production of smoking materials.

In summary, the GM bacteria presented in Table 5-8 may be suited for application under contained conditions. However, transfer of transgenic DNA to natural populations is likely upon discharges from production facilities. Stability of transgenic DNA may be improved by insertion of the *pha*-producing genes into bacterial chromosomes. GM plants presented in Table 5-8 still carry antibiotic resistance markers making them unlikely for production in open fields. The presence of *pha*-producing genes in the cytoplasm is more favourable because sexual exchange of transgenic DNA will be excluded in this way.

Reference and possible application	Host species	Origin of *pha* gene	Other recombinant genes[1]	Location in genome
White Biotechnology				
Fukui and Doi, 1997, 1998	*Ralstonia eutropha* PHB$^-$4 β proteobacterium	*pha*C_{AC} from *Aeromonas caviae* (present name *A. punctata*)	Genes from RSF1010 including streptomycin and kanamycin resistance and *mob* genes	plasmid
Lu et al., 2004	*Aeromonas hydrophila* CGMCC 0911 γ proteobacterium	Acyl-CoA dehydrogenase gene (*yaf*H) from *E. coli*	Genes from plasmid pBBRH including Km resistance and *mob* genes	plasmid
Han et al., 2004	*A. hydrophila* 4AK4	*pha*PCJ genes from *A. punctata*	All constructs possess genes from broad-host-range plasmid pBBR1MCA-2, including kanamycin resistance and *lac* or native *pha* promoter	plasmid
Terentiev et al., 2004	*Arxula adeninivorans* yeast	*phb*A, *phb*B, *phb*C from *R. eutropha*	Genes from plasmid pAL-HPH1 from A. adeninivorans including *hph* gene from *E. coli*, *PHO5* terminator from *Saccharomyces cerevisiae* and ampicilin resistance gene	plasmid
Both				
Romano et al., 2003	*Solanum tuberosum* Potato cell suspension	*Pha*-C1 gene from *Pseudomonas oleovorans*	kanamycin resistance gene	chromosomal
Green biotechnology				
Wróbel et al., 2004	*Linum usitatissimum* Flax	*phb*A, *phb*B, *phb*C from *R. eutropha*	35S (CaMV) and 14-3-3 (potato) promoters and hygromycin resistance gene	plastid
Arai et al., 2004	*Nicotiana tabacum* Tobacco	*phb*A, *phb*B, *phb*C from *R. eutropha*	Spectinomycin resistance gene	plastid

Table 5-8: Genetically modified polyhydroxyalkanoates (PHA) producing micro-organisms and plants

5.2.5 Conclusions

Based on the mechanisms occurring in White Biotechnology and Green Biotechnology as discussed in the previous sections we now draw the following conclusions:

- Production of bulk chemicals by GM micro-organisms in contained facilities (White Biotechnology) is safest with respect to transmission to nature and agriculture.
- Safe containment and inactivation of genes is very important because not all possible implications caused by the release of genes can be foreseen as a result of the complexity of the mechanisms and interrelations involved.
- Particular attention will have to be paid to potential risks related to the management of large volumes of reactor wastes containing living GM micro-organisms. Adequate risk considerations will have to be applied here.
- Current production of bulk chemicals in GM plants (Green Biotechnology) is less accepted due the high chance of transgenic DNA transmission to other agricultural fields or the environment.
- New technological developments aimed to exclude spread or genetic exchange of transgenic DNA from GM plants to other populations make Green Biotechnology a realistic option for the future.
- Transgenic constructs (micro-organisms and plants) containing PHA do not pose rational threats to nature or human health because PHA is a naturally occurring, rapidly biodegradable compound; however, current constructs require further optimization with respect to restrictions on gene flow and absence of antibiotic resistance markers.
- Present-day knowledge on the impacts of GMOs to nature and human health is based on greenhouse and small-scale field trials. Experimental trials for longer periods at larger scale require further exploration.
- Lack of sufficient ecological baseline knowledge limits more precise risk-assessment of effects related to GMO releases.

In conclusion, the risks related to the use of genetically modified organisms in White Biotechnology are manageable if adequate precautionary measures are taken. In view of existing knowledge gaps, the specification of these measures requires further work. The challenges are larger for Green Biotechnology. White Biotechnology is hence closer to large-scale production in chemical industry.

6. Public and stakeholder perception[105]

An important determinant for the success or failure of a new technology is how the public perceives it. For example, the creation of a negative public image of nuclear power following a few catastrophic accidents and the association made by the public between nuclear energy and nuclear weapons has been a major barrier to the advancement of nuclear power in Western countries.

The public perception of the risks associated with a new technology is often unrelated to scientific risk assessment, as the former incorporates value judgements, social norms and traditions that are irrelevant to professional risk assessment.[106] This is likely to be the case also for White Biotechnology.[107] The scope of this Chapter is therefore to discuss the factors influencing public perception and to provide evidence (though limited) of potential obstacles to public acceptance. Due to the limited availability of information we are, however, forced to draw conclusions on the basis of analogies with other technology areas and studies with somewhat different scope and, moreover, to make use of insights collected from a survey among stakeholders (especially from chemical industry) instead of the general public (see below).

In order to set the scene, we begin this chapter with a historical overview of the role of public related to the introduction of new technologies (Section 6.1). In Section 6.2, we provide a literature-based overview of key factors that are expected to determine the public perception of the application of biotechnology for the production of bio-based organic chemicals. In Section 6.3 we discuss earlier studies which allow to draw some first conclusions about the public perception concerning the production of bulk organic chemicals produced from renewable feedstocks by means of biotechnology (these are referred to as "bio-based chemicals" in this report; see introduction and glossary). The results of a survey conducted among EU stakeholders is presented in Section 6.4, which is followed by our conclusions on the public perception in Section 6.5.

[105] The main authors of this chapter are Dr. Fabio Terragni and Dr. Elena Recchia, Centro per l'Educazione, la Ricerca el'Informazione su Scienza e Societa, Milan, Italy. Co-authors of this chapter are:
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[106] The OECD introduced the widely used distinction between *acceptability* of biotechnology related risks, which is linked to a quantitative treatment of accidents probability and which is to be considered as the base for regulation, and *acceptance* of biotechnology risks, as referred to the real social dynamics, not depending on the same "rational" attitude

[107] While the main focus of this study is White Biotechnology, a few chapters (including this one) discuss also Green Biotechnology for comparative purposes.

6.1 Looking back on the role of public related to the introduction of new technology

After the Second World War science and technology were surrounded by great optimism accompanied by trusting deference to scientific experts. Since the late 1960s, several factors began to undermine such unconditional public support to science and to technological applications: a growing awareness of the "dark side" of industrial development (stimulated by isolated warnings such as that contained in Rachel Carson's *Silent Spring*) led to the birth of early environmental movements protesting against pesticides and pollution caused by an unwise use of chemical products in agriculture. At the same time, the status of science as a source of authority due to its neutral and objective character was challenged by the sociology of scientific knowledge.

Following also the seminal work by T.S. Kuhn, *The Structure of Scientific Revolutions* (1970), social scientists analysed the social context of production of scientific knowledge seeking explanation for the different positions that had emerged in scientific controversies, arriving to support the hypothesis that in spite of the standard means of accrediting scientific knowledge as merely objective (experiment, peer review and publication), it has an irreducibly social dimension. This means that the production of scientific concepts is inevitably influenced by the way scientific knowledge has been produced (the organization of scientific work), by the cultural context (and the most widely used images and metaphors), by the economic context (economic interests influence the resources allocation in research), sometimes by the political context (in few instances science has been submitted to political and ideological power).

Recent papers by Sheila Jasanoff (1997) on experts' delivery of opinions (in courts, in federal agencies, in technical-scientific committees) led to the conclusions that consensus over scientific "facts" is often reached through complex negotiation processes (see below).

The public awareness of the risks associated to technological progress was fostered by a series of major accidents (Three Miles Island, Seveso, Bhopal) and, according to some authors,[108] the social dynamics stimulated by the risks associated to technological progress are characterising the present era.

This new awareness of the degree of uncertainty and risk involved in any decision about science and technology resulted in different approaches expressed by various interpretations of the precautionary principle. This concept was developed in the late 1980s. The rationale of the precautionary principle is that it is better not to postpone any precautionary measure to reduce the risks possibly associated to a new technology or product even if there is no evidence of the real dimension of such risks; this interpretation has often led to the situation

[108] This is the thesis developed by the German sociologist Ulrich Beck (1992) in analysing the transition from the modern *Industrial Society*, in which technical knowledge is considered providing certainty and objective knowledge, to the postmodern *Risk Society* where the accumulation of wealth has a side effect a higher social sensitivity to any potential discomfort generated by innovation and a lower tolerance of the risks associated to technologies.

that *the action was not carried out* and to several discussions about the effectiveness of such a principle; to clarify the way it has to be applied, the European Commission issued an official interpretation in February 2000 (Eur. Commission 2000).

In the 1990s, cases such as the BSE crisis and the HIV-contaminated blood have reinforced the suspect that sometimes science and technology can create unmanageable risks (or, even worse, that behind institutional statements and decisions there may be interests in conflict with the public good), undermining further the public trust in scientific and regulatory institutions. These were among the main factors contributing to spread public alarm concerning GMOs release in the environment after 1996, when the first imports of transgenic seeds reached Europe from the USA. The eroded credibility of the institutions in charge of managing scientific and technological developments directly affected the social acceptance biotechnology applications. The term "trust" became a key issue in opinion surveys on the public perception of biotechnology (Eurobarometer on Biotechnology 2002, i.e. Gaskell et al. 2002).

To deal with such crisis of trust, two types of responses have been adopted by public institutions; they can be labelled as "education" and "consultation", respectively.

The first approach tends to identify the crisis as a consequence primarily of public ignorance of scientific knowledge. Education can therefore help to overcome "irrational" fears of new technologies and to win back public trust. However, by failing to address public concerns, the "education" approach may prove to be counterproductive and sometimes result in exacerbation of the trust crisis.

The second approach characterises the crisis as resulting from a lack of public confidence in the involved institutions and stresses the need to re-establish the legitimacy of the innovation process by paying attention to public concerns and demonstrating to take them seriously. This means implementing transparency of regulatory processes and frequent consultation of the public (through several stakeholders).

In the first approach, scientific knowledge is considered as a sufficient source of legitimacy, while in the second the problem is diagnosed as one of political legitimacy: here non-expert (lay) opinions are considered relevant and not dismissed as "irrational", as in the "education" approach, but still distinct qualitatively from expert opinions. A hierarchical division is maintained between "soft" opinions and "hard" scientific basis; while "facts" are susceptible of being assessed in a scientific, objective way, opinions are subjective and value-laden. However, like scientific facts, also lay opinions are obtained through a deliberative weighing of evidence, though not in a disciplined way. This is the reason why even this second approach has been criticised by authors such as Brian Wynne (1995) and Sheila Jasanoff (1997), in the perspective of the discipline of Science and Technology Studies (STS). Instead of considering science as a system of abstract knowledge, the STS approach envisages science as a system of practices embedded in a social and political context. Once the problem of public perception is considered in this broader perspective, public concerns are not limited to factual risks to human health and the environment, but are allowed to encompass broader moral, social and political hazards: for example in the agrofood GMO controversy, risks to the consumers' right to choose, risks for farmers (especially in poor countries) due to the increasing concentration of power and control of food production by a few multinational companies, risks for animal welfare and so on.

According to this perspective the scientific assessment of risks - the objective process of risk quantification as opposed to subjective evaluation - though necessary and useful, cannot provide alone all the answers to the fundamental questions posed by a novel technological application. A narrow framing of risk may facilitate the task of reassuring the public opinion about some of its concerns - but perhaps not the most fundamental.

Moreover, a feeling of powerlessness in the face of technological developments driven by external forces may increase further the perception of risks. Studies of the public perception of risks associated with air travel have revealed that air passengers' lack of control over their environment is the reason why aeroplanes are felt as more risky than cars. This point has been made by the authors of the PABE (Public Perception of Agricultural Biotechnology in Europe) study (CSEC 2001):

"Our hypothesis is that public concern about technological, health and environmental risks is heightened by lack of agency. When people feel that they cannot affect any change within their national political system, they may feel more at risk whilst expressing less apparent concern"'.

Independently of the approach chosen to deal with the public perception of the risks associated to a new technology, there are no doubts that such dynamic is able to determine the final success or failure of a new technology or product. Even the absence of "voice" by the public is not necessarily a reassuring sign: public silence may give the impression of public acceptance, but it may rather reflect a temporary distance form the problem or a deep concern obscured by fatalism, concern that might emerge unexpectedly later, following occasional accidents.

So, it is wise – especially when the involved technology/product is in one way or another linked to biotechnology – to consider properly and *ex ante* the possible response of the public to innovations and eventually address the factors potentially affecting such reactions.

In the following subsections, it will be analysed whether the cited concerns may also be relevant for the biotechnological production of bulk chemicals from biomass, and whether it should therefore be proactively taken into account in the further development of the technology.

6.2 Overview of key factors shaping public perception of the application of biotechnology for the production of bio-based organic chemicals

In this section, we provide an overview of key factors that are expected to determine the public perception of the application of biotechnology for the production of bio-based organic chemicals. We thereby distinguish between "Environmental effects and ethical considerations", "Socioeconomic and macroeconomic effects" and "Incidents" (see subsection 6.2.1-6.2.3). An overview of the key factors belonging to these three categories is given in Table 6-1. For each of the key factors we have collected information that is not directly related to White Biotechnology but which refers to other technology areas (e.g. bioenergy) or impact categories. We use this information to draw first conclusions for White Biotechnology. The outcome per aspect is given in brackets in Table 6-1 and will be discussed in Section 6.2.4.

Environmental effects and ethical considerations	**Socioeconomic and macroeconomic effects s**	**Incidents**
Sustainability of agricultural practices (-)	Security of supply and independence from oil imports (+/0)	Trust as ineludible condition (0/-)
Impact on biodiversity (-)	Redistribution of power between societal actors (-/0/+)	Level of scientific understanding (-)
Land use (0/-)	Influence of trust in the industry and other concerned actors (-)	Existence of preventive measures (0)
Greenhouse effect and fossil energy use (+)	Influence of trust on the development of biomass plants at local level (-)	Workers' safety (0)
Water consumption (-)	Importance of appropriate siting of biomass plants at local level (-)	Fear of terrorists attacks (-/0)
Alternative use of biomass (0 or - depending on alternative)	Job creation and competitiveness (+/0)	
Waste disposal (+/0)	Plant size (-/0)	
Non-productive functions of the countryside (-/0)	Consumers' perception of usefulness and risks of final products (0)	
GMOs (general) (-)	Ethical evaluation (+)	
GMOs in agriculture (-)	The role of the media (0)	
Level of scientific understanding of GMO impacts (-/0)	Price of final product (now -/in future possibly +)	

Table 6-1: Key factors expected to shape the public perception of the application of biotechnology for the production of bio-based organic chemicals

6.2.1 Environmental effects and ethical considerations

The European public showed in several instances to be very sensitive to environmental issues. Such sensitivity has been recently proved by the Eurobarometer, carried out in November 2004, exploring the attitudes of Europeans towards the environment. It showed that almost 90% of Europeans believe that environmental concerns should be taken into proper account in decision making. The state of the environment is perceived to influence the quality of life as much as social factors (72%); only economic factors are perceived as slightly more important (78%). The four environmental problems people worry about most are water pollution, man-made disasters (oil spills, industrial accidents etc), climate change, and air pollution.

Environmental impacts are therefore probably a very important factor triggering the acceptability of the large use of bulk chemicals derived from biomass. The global environmental impacts must be evaluated through Life Cycle Assessment (LCA) that inventories a wide range of environmental impacts throughout a product's life cycle. However, it is should be stressed that LCA studies do not address some specific environmental risks such as out crossing of GM crops, neither do they cover ethical, social and economic aspects. Further assessment methods and some judgement are therefore required in order to arrive at an assessment that can cover all key issues.

Sustainability of agricultural practices

Possible negative impacts are in first instance related to pollution from the use of pesticides, herbicides and other chemicals and to soil erosion/loss of fertility due to inadequate cultivation practices (tillage). Genetically modified crops to enhance herbicide resistance raise immediate doubts about their environmental impact. Moreover, non-food crops can imply massive use of chemicals that would not be allowed for food crops where the health of consumers is directly affected. The experience made with soy bean production in Argentina shows that large-scale cultivation in monocultures can result in serious impacts for the environment and human health and also for society (no alleviance of poverty, reduced employment possibilities; Joensen et al., 2005). On the other hand, non-food crops requiring pluriannual plantation might cause less intensive soil erosion than food crops; the net result should be evaluated case-by-case. In general, biomass derived from food crops (agricultural waste) offers an obvious advantage in this sense.

Impact on biodiversity

Agricultural impacts on biodiversity can be divided into impacts on crop biodiversity and impacts on natural (offsite) biodiversity. Intensive agriculture have negative effects on both types of biodiversity. The introduction of large-scale monocultures and the possible contamination of traditional crops due to gene flow from GM crops might threaten the diversity of local crops. Gene flow from crops which have "wild relatives" in Europe (e.g. *Brassica*) could also affect natural biodiversity. As far as food and fodder crops were affected, genetic erosion would make food production systems more vulnerable to pest attacks and weather events associated with climate change. Attention should be paid to ensure that the diversification of agricultural systems is not affected. In addition, the new crops might go to replace existing habitats for wildlife, especially in Eastern Europe.

Land use

Increased land acreage requirements for non-food crops also could be a potential source of major conflict. Non-food crops compete for land with food crops and wildlife habitats. In contrast to other places where biomass crops have been extensively applied (e.g. Brazil), in densely populated EU countries land is scarce and subject to multiple conflicting claims. Though at present the EU agricultural systems are still generating surpluses, the increasing occurrence of extreme weather events related to climate change such as droughts and floods has negative impacts on yields (especially in the Mediterranean regions) and this might in the next future have effects on the price of food products. In combination with a high-growth energy scenario, land-use could possibly become a limiting factor. In contrast, the use of waste and residual feedstocks again presents an obvious advantage. Therefore, the introduction of large-scale non-food crops should be evaluated in the broader context of the future of EU agriculture.

Greenhouse effect and fossil energy use

Reducing CO_2 emissions is one of the most important reasons for substituting biomass for fossil oil as a source of energy and raw materials. It is generally assumed that the carbon dioxide originating from biomass is equivalent to the amount previously withdrawn from the atmosphere and is therefore neutral in terms of its impact on global climate. However, it is necessary to take into account the use of fuel for agricultural machinery (e.g. tractors), the production and use of fertilizers, transportation of the raw materials and the final products and possibly also a loss of plant biomass from the original vegetation (the extent of this loss depends on the crop, on the type of original vegetation which it replaces and on the climatic conditions). These aspects are, in principle, taken into account in life cycle assessments (LCA; the latter point is generally considered as negligible if crops are grown on existing agricultural land while it must be considered if agricultural production requires deforestation.). Following the lines of life cycle assessment, the calculation results on non-renewable energy use (NREU) and greenhouse gas emissions presented in Chapter 3 and 4 show a clear advantages for White Biotechnology products.

Water consumption

Non-food crops also compete with other land uses for water, that could represent an even more serious source of potential conflict. Irrigation requirements would vary according to crop species. Some fast-growing biomass crops (for example, eucalyptus plantations) have high water requirements and might exacerbate water supply crises especially in Southern European areas threatened by desertification.

Alternative use of biomass

Environmental impacts (positive or negative) can be generated depending upon the alternative uses of biomass crops. For example, if biomass derived from the growth of nitrogen fixing plants previously used as green fertilizer are switched to industrial production, this could have a negative impact on both climate (e.g., due to the production and use of fertilizers) and soil conservation. Again different impacts can be expected for the combustion of biomass for heat and power production.

Waste disposal

One of the benefits of some products of the new technology such as the polymer polylactide (PLA) is its biodegradability. As a consequence the post-consumer waste of products made

from this type of material can be treated in composting facilities or digestion plants. This could help to avoid pollution from waste incineration or of huge and persistent landfill masses. Depending on the waste management system it could imply some change of behaviour for the consumers.

Non-productive functions of the countryside

In the EU, the perceived functions of agricultural systems go beyond the mere production of food and non-food commodities; agricultural systems play a fundamental role in soil protection and landscape conservation, and provide recreational opportunities for urban dwellers. Multifunctionality has been identified as the main feature of the future development of agriculture in OECD countries, with agriculture facing up to the mounting costs of farm support (OECD 2002). In order to test public opinions and expectations, several surveys have been carried out, especially in the UK, where the awareness of agriculture-related issues has grown substantially following several food scandals. The results suggest that the public sees a role for farming as a valued provider of non-market (public) goods such as environmental quality, biodiversity and cultural heritage with farmers operating as custodians of rural land. The public might hence be opposed to an increased industrialization of agriculture. If, on the other hand, agriculture keeps its current role or even extends its supply of non-market goods, this poses the problem of how to compensate farmers for providing these services which have no market value.

GMOs

The application of genetic engineering to agricultural crops and bacteria to be freed in the open environment is one of the most controversial development of biotechnology, especially in Europe (together with GM food). The several cases of opposition to experimentation of GMOs and to commercial licensing are paired by evidences of a relevant lack of support to such kind of applications (see Chapter 6.3 and in particular the Eurobarometers on Biotechnology: a series of opinion surveys carried out by the European Commission in 1991, 1993, 1996, 1999 and 2002, e.g. Gaskell et al. 2002) when compared to applications in medicine, pharmaceutics and even industry. This means a very high sensitivity to the possibly associated environmental and health risks, the lack of perception of the weighted social benefits and a severe ethical assessment.

Following the rise of anti-globalization movements on the international scene, the focus of the public debate on biotechnology shifted from safety issues to broader political ones related to the social impact of the increasing industrialisation of agriculture, the concentration of agriculture control in the hands of few multinational companies, the property of genetic materials, the overall environmental impact of such kind of intensive agriculture. The public attention shifted also to the implications of GM food and crops for farmers, Third World countries, and even for the local cultures and food habits of European peoples (a criticism particularly widespread in France and in Italy).

Compared to “red” and “green” biotechnology, which have been largely analysed in public perception studies, “white” biotechnology has been only marginally addressed in opinion surveys and virtually ignored by popular media. The scarce information that is available on White Biotechnology will be discussed in Section 6.3.

Use of GM crops in agriculture (Green Biotechnology)

According to a FAO (2003) report, *“the scientific understanding of the effects of GM crops at the agro-ecosystem remains limited, also due to the limited number of crop seasons and numbers of generations of crop-associated species for which data have been collected so far”*.

In order to assess the long-term environmental effects of GM crops, a number of aspects should be studied: gene flow, changes in agricultural inputs and practices, changes beyond agro-ecosystems (other biota located within common landscapes). Scientific uncertainty on these issues is accompanied by widespread rejection. Opposition against the agricultural applications of genetic engineering has been growing since the late 1990s worldwide, particularly in Europe (while in the USA opinion polls show that the public opinion is generally more favourable) where it led to a *de facto* moratorium of release and commercialisation of GM crops.

The attitudes of the European citizens to biotechnology (support, risk perception, moral acceptability, perceived usefulness) have been explored by the Eurobarometers in a series of opinion surveys (Eurobarometer) commissioned by the European Commission and carried out in 1991, 1993, 1996, 1999 and 2002. The 1999 survey showed a *clear decline of support for biotechnology* in general between 1996 and 1999 in all European countries (excepted Sweden and Austria). Such decreased support was not due to a general tide of pessimism over the social impact of new technologies, but was specific for biotechnology and in particular of GMO applications in the agro-food area. The latest survey (Gaskell et al. 2002), conducted over a representative sample of 16,500 respondents, has shown that this *trend has stabilised*, though with *significant differences in the various countries* (a slight increase in support has been found in all countries with the exceptions of Germany and Finland, where there has been a stabilisation, and Italy, France and the Netherlands which showed further declines). Differences also emerged in relation to gender, age, education, and level of scientific information. Males, young people (under 39), and more educated people in general show a more supportive attitude to agro-food biotechnology compared to women, people over 55 years and less educated people. However, concerning biomedical applications differences are not significant.

The data confirm the existence of a sharp distinction between medical applications of genetic technologies, that are generally regarded as useful and deserving support, and agro-food applications, for which the perception of social risks tends to prevail over perceived usefulness. On average, the respondents from all the countries that called for an extension of the moratorium on the commercial exploitation of GM food (with the exception of Belgium) are opposed to GM crops. However, opposition against GM food products is more marked than against GM crops. In some countries (Belgium, UK, Germany and the Netherlands) the respondents supported GM crops but not GM food.

As a whole, the Eurobarometer results indicate that public attitudes to GM crops and food have stabilised, though they do not allow to understand whether and how the underlying motives have changed in the past years.

Level of scientific understanding of GMO impacts

Several studies have been carried out to assess the environmental impacts of GM crops. While the occurrence of gene flow affecting wild and cultivated relatives has been demonstrated, as well as the negative effects on some beneficial organisms such as insects (Losey et al. 1999), on the whole the level of scientific understanding seems not to be definitive (see also Chapter 4). However, the results of such studies are probably quite relevant for the public debate on GM crops, which at present appears much more influenced by socio-political arguments. More research would be opportune on the implications of contained use of GM organisms and enzymes in industrial plants (for example, the effects on the health of workers of long-term exposure to biological materials, or the environmental effects of the unavoidable accidental releases).

6.2.2 Socioeconomic and macroeconomic effects

Security of supply and independence from oil import

Geopolitical aspects could be seen as a key factor in assessing the growth of bio-based technologies. Biomass offers a domestically-produced, renewable energy source that could replace in part oil imports from outside the EU, ensuring a stable and secure energy supply and improving the balance of trade of member countries. However, it is not automatically true that these considerations represent a priority for most EU citizens. Some clue to the way the European citizens perceive the need to develop biomass-based energy sources is offered by the results of a recent Eurobarometer survey on *Energy issues, options and technology* (Dec. 2002). The results show that while an overwhelming majority (88%) "consider global warming and climate change to be serious problems requiring immediate action", only 30% regards ensuring "uninterrupted energy supplies" as the highest priority for governments (with "protection of the environment and public health" ranking first). This seems to signal that public concern about the security and stability of energy supply is not very important (however, the recent international developments might have changed many people's attitudes). The public opinion appears largely unaware of the full extent of the problems related to energy supply as well as of the need to develop a comprehensive strategy for the future.

Redistribution of power between societal actors

One of the most controversial issues in public debates is the socioeconomic impact involved in the increased control by industrial corporations on agricultural production, regarded by many as threatening farmers' independence and welfare, increasing their subordination through new forms of contractual relationships and the obligation to comply with strict quality standards set by the manufacturing industry. This point concerns the distribution of social benefits and costs of new technologies. The need to support rural economies seems to require special measures, e.g. some form of compensation to pay farmers for the value of agricultural waste products considered as a resource. A related advantage would be a reduction of greenhouse gas production (and, occasionally, of devastating fires) caused by waste burning. A specific case is represented by organic farmers who might suffer economic damages in case of contamination of their crops through gene flow from GM crops. Conflicts of this type have already been reported by the media, mostly in the USA.

Concerns related to unbalanced power relations might also apply to the location of biomass crops and bio-based productions in Eastern Europe, where national governments often have relatively less negotiating power. The introduction of large-scale biomass crops monocultures there (especially if made at the expense of forests and valuable wildlife habitats) could spread alarm among local and international environmental groups, fuelling concerns about corporate practices.

Trust in industry

The success of any message aimed to communicate the benefits and/or the risks of bio-based technologies would be in the first instance influenced by the image of the sender. Therefore, the first relevant factor to be analysed is the industry reputation.

In the recent past, commercial corporations appeared to be relatively little concerned about social and environmental issues. This has significantly changed in recent years. Environmental concerns, by the 1990s have pervaded the economic and political mainstream

making consumers, and correspondingly industries, more sensitive. This process was undoubtedly accelerated by major shocking incidents (such as the Union Carbide's gas leak at Bhopal, India and the Exxon Valdez oil spill in Alaska). Transnational corporations have been blamed for a wide range of behaviour causing social impacts (children labour, anti-union practices, destruction of local communities), environmental impacts (pollution, deforestation, global warming), financial crimes (false budgeting, money laundering, corruption). Environmental groups such as Greenpeace have developed an unprecedented ability to use media power by mounting campaigns of "direct action" and by appealing to the self-interest of Northern consumers as well as to their responsibility as global citizens.

The pressure built up from environmental groups, trade unions, consumer organisations and part of the academic world came to a head in 1992 at the Earth Summit in Rio de Janeiro. The summit programme of action (*Agenda 21*) called on the world's business leaders to cooperate with governments, international organisations and NGOs to promote sustainable development. The summit opened a new phase characterised by an effort by several big corporations including Unilever, British Petroleum and General Motors, to rethink their strategies and to seek form of partnership with NGOs. By 1998, seventeen Fortune 500 companies were working through the Pew Center on Global Climate Change, an initiative aimed at promoting awareness of climate change and reductions in greenhouse gas emissions. In addition, to build their "reputational capital" many companies autonomously developed their own codes of conduct and set standards for corporate social responsibility.

Corporations find increasingly difficult to consider the pursuit of the interests of shareholders as their sole purpose, in line with the argument of neoclassical economists that the only responsibility of business is to make profits (Milton Friedman 1997). Whether as a cosmetic image exercise or as a genuine effort to improve the social impact of corporate practices, the development of responsible business policies has come to be considered by the companies themselves as a key factor of success. This trend has been recently stressed by the UK Chemical Industries Association (CIA). At the 2002 conference of the International Chemical Industry Labour Relations Committee in Bergen, CIA Director of People, Knowledge and Communication, Anil Kumar, stated that by adopting the principles of Corporate Social Responsibility the global chemical industry not only would enhance its reputation, but would also achieve "real business benefits". Indeed previous research had found evidence that firms active in "corporate global citizenship" financially outperformed their competitors.

The increased companies' vulnerability to public criticism is also related to the new NGOs' networking and communication abilities, that allow them to circulate information about the impact of negative corporate behaviour in immediate and timely ways at a moderate cost by using information technologies. Considering the new risk for companies from negative media exposure as well as the increased leverage of NGOs, Ulrich Beck (1992) has defined the latter as "an expression of reflexive modernisation" rather than of backward-looking criticism of scientific and technological progress.

Some indications of the state of industry's reputation in Europe are offered by the Eurobarometer surveys; in the 2002 edition the sample showed to trust in general doctors, academics, and consumers' and patients' organisations. Academic scientists appeared much more trusted than scientists working in industry, with confidence scores of 76% and 56% respectively. As a whole, the results are consistent with those of previous surveys. However, for industry the data shows a sharp improvement between 1999 (when industry had a confidence deficit of minus 10%) and 2002, when it won a 23% surplus. It has been argued that the improvement might be related to increased confidence in national regulations and relatively high confidence in the European Commission, or to the fact that the public's association with the term industry has changed from agro-food to medical biotechnologies.

Asked specifically about biotech, the interviewed answered to trust more the medical profession, followed by consumers' organisations and environmental organisations, university scientists, television and the media. Industry scores very low (only 5%).

The current difficult position of industry is partly resulting from poor communication with the public and failure to understand public concerns. Until 1997-98 the business community largely underestimated public opposition, judging it irrational and due to residual fears that would have gradually faded away. In time, the public resistance to accept biotechnologies has proven qualitatively different from that commonly associated to the introduction of any technical innovation and much harder to overcome. Industry has then tried to take the problem seriously and to react through communication initiatives aimed at promoting the public image of biotechnology, by stressing its possible benefits. In particular, agro-food biotechnology has been presented as the best way to provide sufficient food for a growing world population in the next future. However, some factors have undermined the credibility of this presentation of the problem.

The influence of trust on the development of plants at the local level

Though the perceived uncertainty surrounding the reliability of oil supply from those geographical areas involved in the war to global terrorism may accelerate the obtaining of a general consent to the development of alternative sources, this does not automatically involve the consent to plant development at the local level, where siting controversies are quite common due to widespread NIMBY (*not-in-my-backyard*) attitudes. Many concerns expressed by the residents in the vicinities of plants are the same whatever the technology used. The obtaining of planning consent was identified as the main obstacle to the growth of the renewable energy industry in a survey conducted in 1996 by the UK Association of Electricity Producers (AEP 1996). The methods for dealing with public concerns are crucial, as reciprocal risk communication, interaction with the local institutions and media and stakeholder consultation/participation contribute to increase public trust in decision making (conversely, the lack of communication can accompany poor levels of trust) (Sinclair and Lofsted 2001).

Another crucial condition in planning agricultural crops is the choice of the site (siting). Besides the usual fears (e.g. about possible accidents, pollution and noise), further concerns may arise among residents in specific local contexts. For example, the planning of new plants can face considerable public opposition both in areas where the residents' health and the local environment have been heavily damaged in the past due to the pollution created by other industrial plants or waste disposal facilities, and in intact rural contexts where the new plants can impair the amenity of the landscape (and, consequently, on local tourism) (Bishnu and van der Host 2004). In both circumstances, the site selection of the plant is likely to be viewed as unfair and inappropriate and controversies will probably arise.

Job creation and safeguarding and international competitiveness

A major relevant factor for the social acceptability of bio-based industrial processes (especially at the local level) is their potential in terms of job creation. Employment-related considerations often prove overwhelming in the social evaluation of technologies and single plants, offsetting environmental and other concerns - even when safety and health of the workers themselves are at stake. Given the early stage of development and the extensive need for R&D and implementation and – moreover – the involvement of the agricultural sector, bio-based industrial processes can be expected to create or at least safeguard jobs and to contribute positively to international competitiveness. Since the growth of the bio-based sector will partly occur at the expense of other sectors (in particular, at the expense of the

conventional chemical industry), estimates of the net effects for the job market and for international competitiveness would be required in order to assess the possible importance of this aspect. Moreover, it would need to be taken into account that international competitiveness is generally not valued as positively by the public because companies may be competitive and economically healthy while laying off personnel.

Plant size

The public acceptance of single production plants would probably depend by their size. While large-scale plants for bio-based chemicals could meet opposition by local communities, for their perceived environmental impact, small-scale plants would probably be better accepted as a positive contribution to local economies.

Eurobarometer 2002 on Energy shows that a majority of the respondents wish to be consulted on plans or construction projects in the energy sector, in particular where "local" plans are concerned. This indicates that a general concern about the possible impacts of industrial plants indeed exists. Public concerns might grow following possible industrial incidents, already mentioned as factors that can radically change the public perception of a technology; or as a reaction to inadequate behaviour on the part of public authorities and/or the industry.

Consumers' perception of usefulness and risks of final products

"Useful" could mean "perceived as contributing to improve one's way of life". Indeed many novel products recently introduced can be hardly defined as "useful" in a strict sense. In many cases, social costs may outweigh social benefits. Rational and objective weighing of risks against benefits is seldom determinant to the success of any innovation. Instead, inconsistency often seems to characterise public attitudes (e.g., the same people who enthusiastically welcome the introduction of mobile phones are not so easily willing to accept the location of antennas in their neighbourhood). But while mobiles are very exciting toys for adults and kids, unfortunately, the same cannot be said of the products of biotechnology.

On the other hand, this point is only partly relevant in our case. The production of chemical intermediates from renewable raw materials does not concern directly the final consumer. To improve the public perception of benefits, information campaigns could be carried out stressing the advantages offered by using renewable materials: reducing dependence on oil, improving waste disposal (biodegradable plastics).

A key outcome from Eurobarometer 2002 is that the European citizens do not appear technophobic. The majority of them think that the most significant technologies which emerged in recent years (with the exception of biotechnology that is associated to mixed feelings) will effectively improve their way of life. A general rejection of bio-based production of chemicals based on ideological prejudice, therefore, is not to be expected. The acceptance is rather likely to be product-specific, depending on whether end products are only produced in a different way or whether they have perceivable, altered properties compared with conventional products. Moreover, novel products might require a change of behaviour (e.g. biodegradable plastics which must be disposed of differently from conventional waste). Also the image of the product may play a role (whether it is perceived as "polluting"), and this characteristic may be altered through biotechnology.

Risk perception is a major factor in the consumers' "cost-benefit analysis". The concept of "uncertainty" is considered by some authors (CSEC 2001) more relevant than "risk" for the public acceptance of new technologies. The results of Eurobarometer 58.0 on biotechnology (Gaskell et al. 2002)reveal that a majority of the European citizens consider GM crops as "risky"; however, this does not involve automatic rejection (thereby accepting uncertainty as a fact of life).

The perception of risks for human health involved in the consumption of specific bio-based products appears a critical issue only as far as they enter the food production chain as ingredients, additives or adjuvants. Other products (biofuels, bioplastics, industrial intermediaries for non-food products) *might* well involve unknown risks, but they seem not susceptible of raising specific concerns among the consumers given the present state of knowledge.

Ethical evaluation

Ethical factors are another relevant factor in consumer choice. Evidence that many people are willing to pay more for products that meet given ethical standards is offered, among other things, by the increasing sales of fair trade products in Europe. Recent data again give us a clue in this respect. One of the most persuasive reasons for buying GM food indicated by respondents is "environmental benefits" (following health benefits due to absence of pesticide residues). Though it is likely that in some circumstances people are thinking as citizens rather than as consumers and that their statements are not fully consistent with actual behaviour, the fact that ethical judgement ranks among the most important motivating factors suggests that we should take it seriously.

The role of the media

The media clearly play a role in the way a new technology is framed by the public and in the social amplification of risks. However, blaming "sensationalist reporting" for biased public perception is misleading. Media coverage can only amplify the public fears, in a cumulative process whereby public and media interest reinforce each other; it cannot create them. It has been argued that any media coverage of scientific controversy, whether positive or negative in tone, by focusing the attention on risk, results in negative public opinion. But, as Dorothy Nelkin (1995) points out, there is no single relationship. Though the media represents a major source of information on scientific and technological developments for most people, its influence on public opinion may vary according to the audience's interest and experience. At least in the case of the GM controversy, a responsibility of the media in *generating* public anxiety has to be excluded, because it was scientists, not the media, who first pointed to the hazards involved in the novel technology. Most studies of the public perception of risks do not consider the media role as a key factor.

Price

A key factor to assess the potential acceptance of final products from renewable energy sources is their price (compared with that of conventional products). This point is particularly relevant for biofuels. At the moment, the production cost of biofuels are consistently above conventional petroleum-based fuels. The per-litre price difference between pure biodiesel (i.e. of 100% agricultural origin) and fossil diesel oil ranges about one-third. However, this aspect should be evaluated by taking into account current trends of energy price indicating that the days of cheap energy are ended. In addition, in order to encourage the consumers to change their purchasing behaviour, governments can implement tax measures - for example reducing or exempting excise duties on biofuels, mainly biodiesel, as already happened in France, Italy, Sweden and the UK - or regulations setting a minimum percentage of biofuels in commercial transport fuels. The Green Paper entitled "Towards a European strategy for the security of energy supply" (Eur. Commisss. 2002) stressed the key role of tax instruments in reducing the price differential between biofuels and rival products.

6.2.3 Incidents

Originally, the term "contained use" was only used to designate use of GMOs in research laboratories, but for the last ten years or more modified organisms have also been used within industrial environments where the volume of material is considerably greater and the personnel handling the organisms may be less knowledgeable and competent. This implies a higher risk that *accidental* escape may occur in a volume great enough for GMOs to survive and persist in the open environment. There is also a risk of *incidental release* via waste streams or rubbish if waste from the industrial plant is not adequately monitored or controlled. The potential risks for human health posed by large-scale fermentation of GMOs include:

- infection hazards - the potential for disease following exposure to the organism;
- toxic, allergenic or other biological effects of the non-viable organisms, its components or its metabolic products;
- toxic, allergenic or other biological effects of the product expressed by the organism.

Under conditions of "Good Industrial Large Scale Practice" (GILSP) established by a working group of OECD (1986) the host organism must be non-pathogenic to humans and with an extended history of safe industrial use; the modified organism must also be non-pathogenic, but with limited survival in case of unwanted release into the environment; and the vector must be well characterised, free from known harmful sequences and unable to transfer any resistance markers (anyway, the practice of including of antibiotic resistance in GMOs has been virtually abandoned).

Independently of the severity of their consequences, accidents are the signal that systems are susceptible of failing and may spread the concept that technology is out of control. Major industrial incidents can radically change the public attitudes to a specific technology. The most obvious example is the impact of Tchernobyl disaster on the public perception of nuclear energy plants in Italy which led to a ban on nuclear energy production on the national territory. Though such reactions may appear irrational and disproportionate, the public evaluation of risks is only partly based on the scientific definition of risk – probability times severity of harm – but is shaped by a complex set of supporting circumstances or qualitative factors (often tied to symbolic attributes more than to the actual advantages and disadvantages of a specific risk source), that have been identified by a number of studies (e.g. Slovic 1987). These cannot be simply dismissed as ignorance, though the inability of many people to understand probabilistic statements, or to recognize risks from familiar sources, might lead to such a conclusion, thus supporting the idea that education and (one-way) information can remove the problem (Renn and Levine 1988). However, the so-called "fright factors" often reflect fundamental value judgements. Most studies of risk perception agree that trying to reassure the public by some "quick PR fix" will therefore ultimately undermine reciprocal trust and institutional credibility, while successful risk communication strategies should rather rely on *long-term* commitments to openness, transparency and dialogue.

People's attitudes towards risk are basically of individual character and their preferences are often inconsistent. However, several studies have shown that, regardless of their social and cultural background, people everywhere apply practically universal risk assessment criteria (Renn and Rohrmann 2000) and have identified some of the most influencing factors in the social/individual acceptability of risk:

i) *Voluntarity*. People are more willing to accept risk when exposure is voluntary (as in dangerous sports or smoking) than when they are forced to run it by others.
ii) *Fairness*. Risks are better accepted when benefits and eventual costs are equitably distributed.
iii) *Familiarity*. People are more reluctant to accept risks arising from unfamiliar sources.

iv) *Scientific uncertainty*. Risks which are poorly understood by science are generally more worrying.

The latter two factors will clearly be relevant in any case to the perception of the risks of what is an entirely novel technology, while the first two will be conditioned by the fundamental social options accompanying the future development of the industry.

Trust as ineludible condition

What has been said above about the influence of trust on the public acceptance of plants under normal operating conditions is even more relevant as far as possible accidents are concerned. A recent event may reinforce this conclusion, though it was only a minor mishap without apparent implications for human health and the environment. On 17 and 18 August 2004, two accidental releases of materials containing genetically modified organisms took place at the Novo Nordisk production site in Bagsværd, Denmark. According to the company report, "During a transfer of liquid from a tank to a truck approximately 500 litres of water containing approximately 3 ml GMO liquid from a laboratory was accidentally let to the rainwater drainage". The social amplification of this event in terms both of (international) media coverage and public reactions has been very scarce. This can be explained by two basic considerations: 1) it appears as a further confirmation that the contained use of GMOs is intrinsically less controversial than open field applications (GM crops) and 2) it may be seen as a demonstration of the success of a risk communication based on openness and dialogue which has traditionally characterised Novo Nordisk's strategy, in contrast to "risk minimizing or simply denying" approaches adopted by other organisations.

Needless to say, in case of eventual accidents any attempt to conceal the facts to the public opinion, when disclosed, would definitely destroy the public trust not only in the concerned organisation, but in the entire industry.

Level of scientific understanding

The present level of knowledge of the possible impacts of GM bacteria/enzymes releases in the environment seems absolutely insufficient (compare Chapter 5). No plant safety claim will appear entirely credible until the scientific state of the art is not substantially improved. The development of the industry must be accompanied by adequate public and private research e.g. on GMO survivability and persistence, changes in soil ecology due to GMO releases etc.

Existence of preventive measures

A key condition to prevent possible damages from accidental GMO releases is that the organisms are designed so that they are not able to survive in the open environment. The GMOs which were accidentally released at Bagsværd could not survive outside of the protected environment in the laboratory. It is therefore unlikely that the GMO cells could spread to the external environment and be harmful to humans and the environment.

Workers' safety

The first group which could be harmed by eventual accidents is workers. Even if the external environment and the local population were unaffected, any serious damage suffered by the workers following an accident at some plant would have negative effects on the image of the plant in question and, most likely, of the whole industry.

Fear of terrorists attacks

In principle it is conceivable that industrial facilities were attacked causing widespread release of GMOs in the environment with unpredictable consequences. At least so far, the terrorist strategies have been focused on direct destruction of human lives and buildings by (more or less) conventional weapons, rather than on disrupting the target societies by causing widespread contamination with dangerous (chemical or biological) substances. However, though implausible, it is an eventuality to take into consideration. It reinforces the requirement that processing plants only use organisms that are unable to survive in the external environment.

6.2.4 Summary of first assessment

Using information that is not directly related to White Biotechnology, we conducted in this Section 6.1 a *first* assessment of the factors shaping public perception of White Biotechnology. The outcome per aspect is given in brackets in Table 6-1 and can be summarized as follows:

- Aspects that can be expected to contribute positively to the public perception of White Biotechnology are the low greenhouse gas emissions and fossil energy use, waste disposal, the contribution to the security of energy supply, the positive effects for job creation/safeguarding and competitiveness and some ethical considerations.
- All other aspects (see Table 6-1) are expected to be either neutral or to contribute negatively to the public perception of White Biotechnology.

The number of factors rated neutrally or negatively is quite substantial. In order to arrive at an overall conclusion about the public perception of White Biotechnology, the individual aspects would therefore need to be weighted. Since the information required for this purpose is not readily available we pursue in the next two sections (Section 6.3 and 6.4) other approaches in order to arrive at overall conclusions (Section 6.5).

6.3 The outcome of earlier studies

A comprehensive search of existing studies of public perception focused on White Biotechnology was carried out. None of the five studies found deals exactly with the subject matter of the BREW study which aims to obtain insight into the public perception of the wide range of White Biotechnology products and processes in Europe. The studies found mostly deal with a relatively small product area within White Biotechnology (especially plastics) and specialties within this area (biodegradable plastics). Moreover, three of the five studies analyze the situation in Germany which may not be representative for Europe. Nevertheless the five studies found contribute to a somewhat clearer picture of the factors that are relevant for the public perception of White Biotechnology:

- The Eurobarometer surveys on biotechnology (Gaskell et al. 2002; INRA/ECOSA 2000) are interesting because they cover several aspects and applications of biotechnology (even if White Biotechnology is cited only once) and because they are European wide.

- The German study *Technology acceptance and demand patterns in plant biotechnology* (Voß et al. 2002 see below) which is limited to Germany, deals with various types of applications for Green Biotechnology for the production of chemicals in agricultural crops (PHA producing crop plants); this only plays a minor role in the BREW study.
- The pilot project carried out in Kassel, Germany (Lichtl 2003; Käb et al. 2002), is much more specific but covers only biodegradable plastics which represent only one category of products that can be produced by application of White Biotechnology (other categories are non-biodegradable plastics and other organic compounds apart from plastics); moreover, biodegradable plastics can also be produced in other ways apart from White Biotechnology. The pilot project is anyhow interesting, as it does not only ask for preferences and attitudes but probes actual behaviour of involved players, especially consumers.
- An international study commissioned by Cargill Dow (now: NatureWorks) provides additional insight on biodegradable plastics for food packaging (NatureWorks 2003).
- Finally a rather old German survey (Meinecke & Rosengarten 1996) on renewable resources is reported because it covers biomass use for industrial products.

6.3.1 Eurobarometer survey

As explained above (see Section 6.2.1) the Eurobarometer surveys (Gaskell et al. 2002; INRA/ECOSA 2000) show a decreased support for biotechnology in general between 1996 and 1999 followed by stabilization at a low level of acceptance. This development was mainly shaped by the developments in the agro-food sector (Green Biotechnology). No one of the questions in the latest Eurobarometer (Gaskell et al. 2002) concerned the industrial non-food, non-medical applications of biotechnology. However, the results of Eurobarometer on Biotechnology 2000 (INRA/ECOSA 2000) offer limited insight to assess the social acceptability of bio-based industrial non-food applications. One of the six applications of biotechnology evaluated by the respondents, namely enzymes produced with genetically modified organisms and used for environmentally friendly detergents, is judged to be useful and supported by a majority. This indicates that White Biotechnology, involving a benefit for the environment, may be well accepted even when genetic modification is involved.

6.3.2 BMBF Project in Germany

Funded by the German Federal Ministry of Education and Research (BMBF), a research project on "Technology acceptance and demand patterns in plant biotechnology" was carried out in Germany in 2001-2002 by the Technical University Wildau (Voß et al. 2002). Within this project, a locally restricted internet survey was carried out from October to November 2001, targeted at internet users in the Berlin-Brandenburg region which covers both urban and rural residents in Western as well as Eastern Germany. A total of 201 analysable responses were received. The socio-demographic data of the respondents were typical for internet users (and thus different from the general public).

The survey comprised three parts: in part 1, respondents were asked to assess genetic engineering of agricultural crops (Green Biotechnology) in general and if applied to different applications (food use, input traits, use as feedstock for industrial products) and to give reasons for their assessment. In part 2, a defined innovation project, namely the production of biodegradable plastics in genetically modified plants was to be assessed in a similar way as the options in part 1. In part 3, it was investigated whether the assessment of the innovation project is influenced by knowledge of possible impacts of the innovation. For this purpose, comprehensive and unbiased information of possible impacts were provided, covering all relevant impact dimensions. Respondents were asked to reassess the innovation project in the light of the additional information privided and to give reasons if their second assessment diverged from the initial one. All in all, the following results were obtained (Figure 6-1 to Figure 6-3):

- A global rejection of plant genetic engineering in general or of different applications, as often reported in the media and by stakeholders, could not be substantiated with this survey: For four of the five items on genetically modified crop plants, positive attitudes prevailed over negative ones. The only application assessed negatively by the majority of respondents was the genetic modification of crop plants for food purposes. Roughly one fifth of the sample was undecided in all five cases (Figure 6-1).
- Respondents clearly differentiated between different applications of Green Biotechnology: Only green Biotechnology for food production was assessed negatively by the majority in the sample. , Green Biotechnology with improved input traits scores more or less equal with plant genetic engineering in general (without specifying any applications or uses), and Green Biotechnology as feedstock for industrial purposes as well as the genetically modified plants producing bioplastics were assessed as the most positive option.[109]
- Environmental (ecological) and health are the most important factors for the respondents' assessment, with health reasons being most important for food use, whereas environmental reasons prevail in the assessment of the other applications. All in all, Figure 6-2 shows that there are application-specific patterns of reasons which are important for the assessment.
- In the assessment of the specific innovation project (Green Biotechnology for the production of biodegradable plastics), positive attitudes prevailed significantly over negative ones (64% of respondents vs. 16%, 19% being undecided), and environmental reasons were most important for this assessment (given by 74% of all respondents). Remarkably, economic reasons (competitive advantage (39%) and employment effects (32%) were given by approximately one third of all respondents – no other option received such high rankings in these categories (Figure 6-2). The assessment of this innovation project was influenced by knowledge of its possible impacts (Figure 6-3): while 69% of the respondents sticked to their initial assessment even after they had been given information on possible impacts, 31% changed their opinion. The majority of the persons who changed their assessment (including gradual changes) developed more positive attitudes (21% of all respondents). Figure 6-3 gives an overview which changes in opinion were recorded in detail. Although the subsamples of the respondents who changed their assessment are too small to draw statistically significant conclusions, there seems to be a tendency that impact knowledge primarily reinforces previous assessments (rather positive/negative assessments become strongly positive/negative), and, to a lesser extent,

[109] No information from the original study is available whether the slight differences in the assessment of the industrial feedstock option and the bioplastic from genetically modified plants are significant or not.

supports undecided respondents to develop a clearer (positive/negative) opinion. By contrast, *drastical* changes from positive to negative assessment or vice versa through impact information seem to be rare. The majority of the respondents (59%) were interested in further information on the innovation project in order to back up their assessment. Respondents asked for more information on further impacts of the use of such genetically modified plants (83%), whereas "technology information" on the applied genetic engineering methods and the properties of the modified plants were of lower importance (45-50% of respondents).

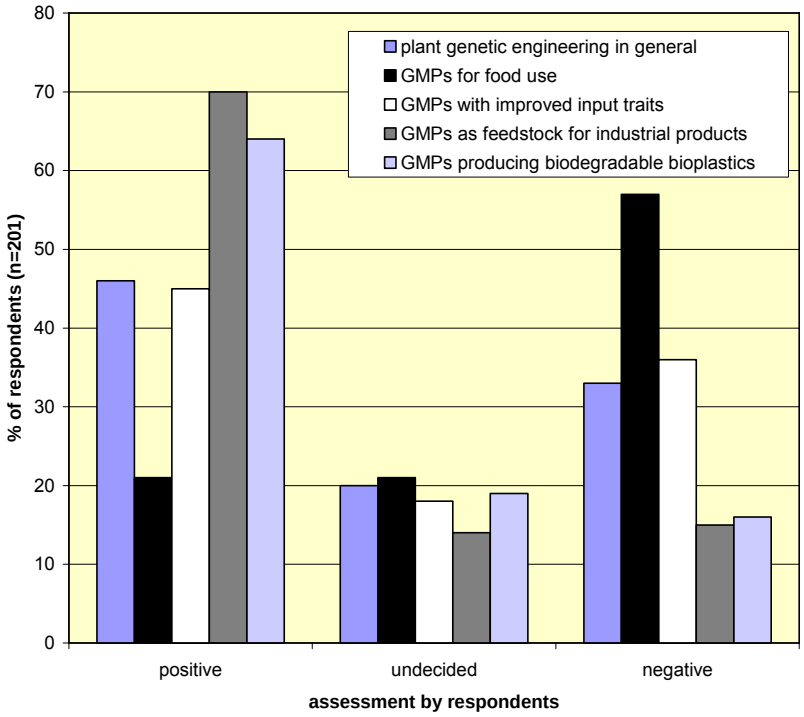

Figure 6-1: Assessment of plant genetic engineering in general and different applications by respondents to an internet survey in Germany, 2001 (Voß et al. 2002)

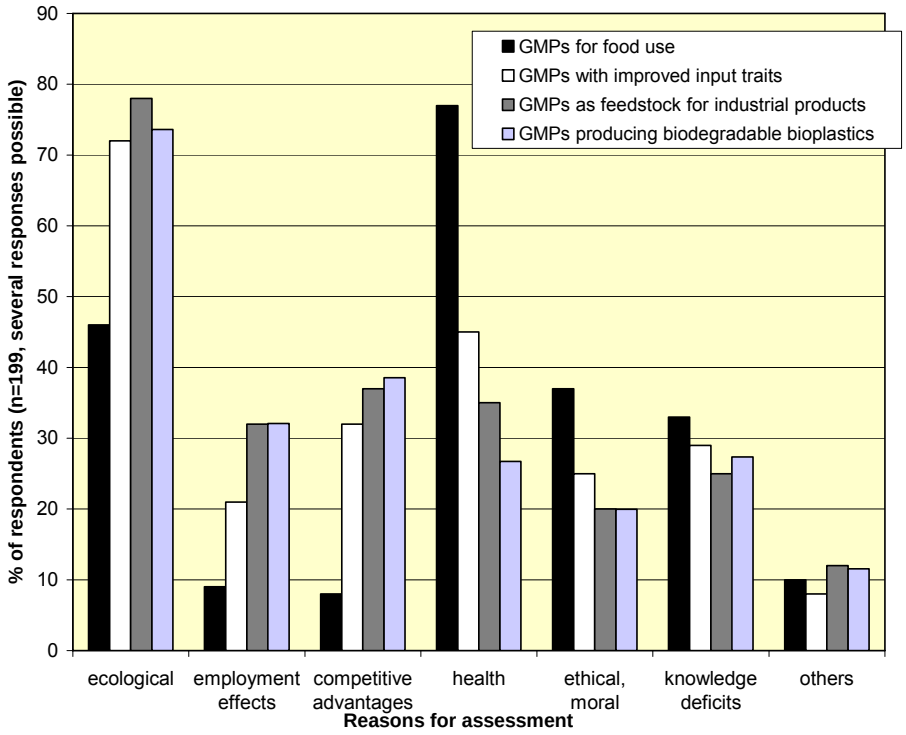

Figure 6-2: Reasons for the assessment of plant genetic engineering and different applications, as given by respondents to an internet survey in Germany, 2001 (Voß et al. 2002)

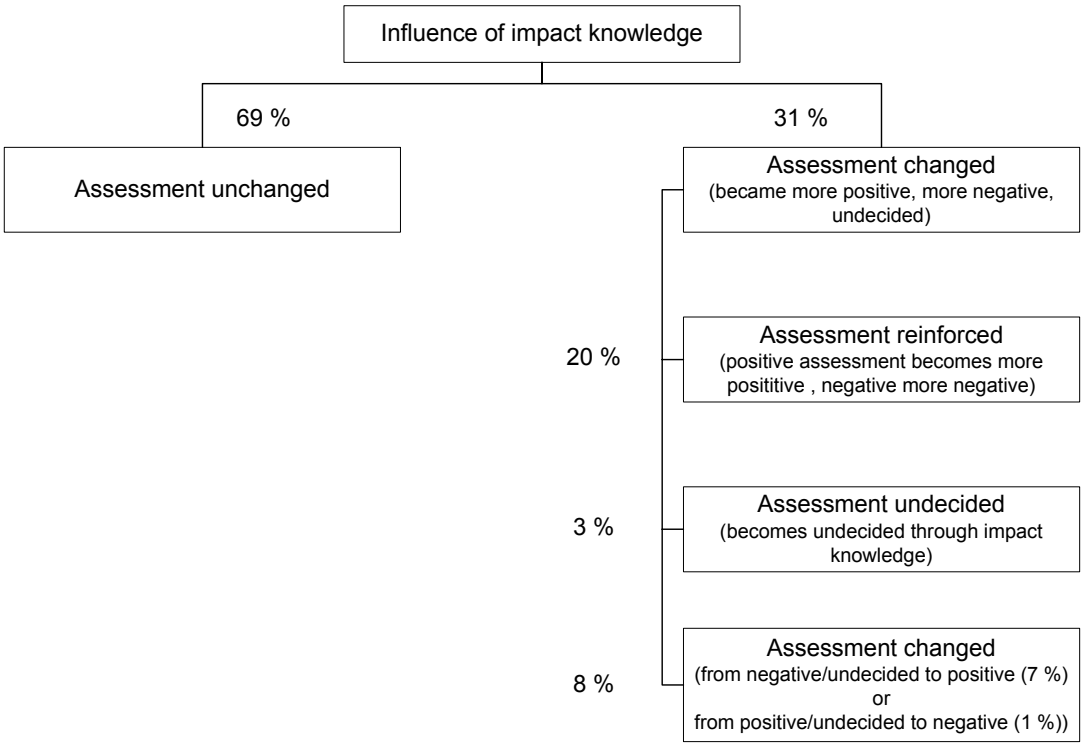

Figure 6-3: Influence of impact knowledge on the assessment of GVPs producing biodegradable bioplastics by respondents to an internet survey in Germany, 2001 (from Voß et al. 2002)

6.3.3 Kassel Pilot Project

A pilot project for marketing and recycling of compostable packaging made from biodegradable polymers was run in the city of Kassel in Germany (Lichtl 2003; Käb et al. 2002). From May 2001 to November 2002, retail chains in Kassel sold about a dozen products in packaging made from biodegradable - i.e. compostable - materials. In order to mark biodegradable packaging (made of biodegradable polymers), it was marked with a hexagon for easy identification and separation by the consumers. A promotional campaign under the motto “the sixth sense” explained the meaning of the logo with the compostability symbol in its centre to the 200,000 inhabitants of Kassel. It started with house-to-house circulars and was backed up by roadshows in public places and schools, along with notices and advertising campaigns in shops. Kassel’s retailers initially were skeptical due to the pricing of the packaging, but the outcome was so positive that with certain products the use of biodegradable packaging actually led to increased sales.

When interpreting the outcome of this project it should be kept in mind that biodegradable (compostable) polymers can be manufactured not only by means of White Biotechnology and with renewable raw materials as feedstock but alternatively also starting from petrochemical inputs and applying conventional chemistry. Moreover, White Biotechnology allows to produce also chemical products that are not biodegradable. The biodegradable polymers used in the Kassel project were fully or partially bio-based and surveys among the clients revealed that environmental attractiveness was associated to a comparable extent to the use renewable

materials and to compostability.[110] This means that the use of bio-based feedstocks (as it applies to all White Biotechnology products studied in the BREW project) is a key reason for the positive perception. Therefore, in spite of the incomplete congruence, the outcome of the Kassel project has quite some explanatory power also for White Biotechnology products in general. Weak points of this analogy are that overwhelming majority of the interviewees in Kassel was probably not aware of the fact that some of the biodegradable polymers were White Biotechnology products while others were chemically modified thermoplastic starch; moreover, most respondents associated genetic modification with agricultural crops while they were most likely unaware of the *possibility* (this is not a *necessity*) of using genetically modified organisms in the fermentation step of a White Biotechnology process. It is unclear how this additional insight would have altered the results.

The results of the Kassel Pilot Project (Lichtl 2003; Käb et al. 2002) can be summarized as follows:

- The overall results of the survey on the acceptability of biodegradable polymers to consumers, conducted in September 2001 with 600 Kassel citizens, were very encouraging. About 90% considered the idea of replacing conventional plastic packaging with compostable packaging as either good or very good, 80% evaluated the quality of biodegradable polymers as either good or very good, and 87% said they would buy it again. In addition, one third of consumers would be willing to pay a surcharge of up to 15 cents for a compostable carrier bag, instead of the current 10 cents. For a biodegradable yoghurt cup, they would pay an extra 5 cents. Beyond this price limit, however, sales of the new material would encounter serious difficulties.
- When asked to rank packaging materials with regard to their environmental attractiveness, the respondents ranked biodegradable polymers highest (93 points), closely followed by recycled glass (91 points) and paper (82 points). Glass (without recycling) had a medium position (63 points), while composite materials (Tetra Pak, 29 points), metals (16 points) and conventional plastics (7 points) were in the lower range (Lichtl 2003). The amazing result is hence that plastics – in spite of their outstandingly bad image in public - suddenly score highest if they are equated with biodegradable polymers.
- According to the overwhelming majority of the clients (approx. 90%) biodegradable polymers will play a similarly important role as future environmental technology such as solar and wind energy. Given the very positive standing of renewable energy in public perception, this once more confirms the very large environmental benefits associated with biodegradable polymers (Lichtl 2003).
- This outcome is also consistent with the standpoint of the majority (73%) supporting the idea of laws for the promotion of bio-based packaging in order to save oil and strengthen climate protection (Lichtl 2003).
- Around 90% agree that one of the key benefits of biodegradable polymers is to use limited oil resources for more valuable applications than packaging (Lichtl 2003). The respondents hence assume that biodegradable polymers require less non-renewable energy use for their production than conventional polymers. This, however, is not necessarily true because the non-renewable energy use for the production of biodegradable *petrochemical* polymers is similar to that of non-degradable petrochemical polyesters. The concept of biodegradable polymers as understood by the respondents, hence inevitably involves the

[110] Out of a total set of 600 respondees, 18% found the use of renewable raw materials a more convincing argument for the environmental friendliness, 23% argued with compostability and 56% found both features equally important for environmental attractiveness.

production from bio-based feedstocks. This hence represents a good justification for applying findings of the study to White Biotechnology products.

6.3.4 NatureWorks' Graptine study

In Summer 2003 a study on maize-based polylactic acid (PLA) was conducted in the U.S. and in Europe (NatureWorks 2003). The study was commissioned by Cargill Dow (now named NatureWorks). It was performed by the survey specialist Grapentine Inc. to assess the market appeal of natural packaging and consumers' willingness to pay more for compostable packaging material. Within Europe, around 2500 consumers were surveyed in Germany, Italy, France and the UK (about one fourth in each country). According to the survey 59% of respondents found the bio-based packaging concept "very desirable" and about one third of this segment were willing to pay an incremental 20 cent per package of food. Similar results were found by Grapentine Company in Japan: 56% of Japanese consumers ranked the concept of purchasing fresh food in nature-based see-through packaging as *"very desirable."* Of those, more than 57 per cent were willing to pay at least 5 yen (4 Eurocents) more for products packaged in biodegradable containers.

6.3.5 Survey on renewable resources in Germany

In 1996, a representative telephone survey among 1,000 German citizens (age 18-65) was commissioned by the German Agency of Renewable Resources (Fachagentur Nachwachsende Rohstoffe, FNR) to a marketing company (Meinecke & Rosengarten 1996). It was carried out in January/February 1996. The survey was commissioned based on the understanding that the subject "renewable resources" and its role in environmental protection and saving of non-renewable resources is hardly known to the general public, while the development of products from renewable resources strongly depends on the demand for such products. The results of the survey were intended to support the Agency of Renewable Resources in shaping their information efforts according to specific target groups. Therefore, the aim of the survey was to identify and characterise groups in the population regarding

- their general attitude towards environmental issues,
- emotional and cognitive components linked with renewable resources,
- their understanding of the term "renewable resources",
- their knowledge of renewable resources and their fields of application,
- their use of products made from renewable resources,
- their assessments of arguments pro and contra renewable resources,
- sociodemographic factors.

All in all, the survey yielded the following results (Meinecke & Rosengarten 1996): Regarding general attitudes towards environment and environmental protection, there was a high awareness and interest for these issues. Tackling these problems was predominantly seen as responsibility of "everybody" and the government. As a consequence, an environmentally conscious behaviour as well as governmental interventions and sanctions were called for. A positive attitude towards environmental protection prevailed, but should not result in increased costs. Regarding renewable resources, there is a low level of knowledge in the general population. The term "renewable resources" had never been heard or read by 33% of the respondents, and 45% cannot give spontaneously any example of renewable resources or

products derived thereof. Men show a better knowledge than women. The most well-known examples of renewable resources were wood (named by 30% of respondents), rape/rape seed oil (27%), hemp (16%) and natural fibres such as cotton (9%). All other renewable resources were named by less than 5% of the respondents. However, it was not spontaneously known to 70% of the respondents which other resources could be saved by renewable resources. Despite low knowledge of renewable resources, positive attitudes prevailed (Table 6-2). A cluster analysis revealed five different population segments, based on their attitude towards renewable resources. Their key characteristics are given in Table 6-3.

Item/statement	% of respondents with strong agreement[111]	Average agreement[112]
There are not enough efforts to make renewable resources attractive for the consumer	75	no data
It is important that the government supports the production of renewable resources and the sale of products made from renewable resources	77	6.3
The production of renewable resources offers new perspectives for the German agriculture	74	6.2
At present, the population does not know enough about the subject "renewable resources"	73	6.0
If I had the choice, I would choose the product made from renewable resources	71	6.2
Products made from renewable resources are always more environmentally friendly than products from fossil resources	70	6.0
For a product made from renewable resources, if of the same quality as a conventional product, I would pay some more money, as a contribution to environmental protection	64	5.8
Products from renewable resources must not be more expensive than conventional products	63	5.6
Products from renewable resources (e.g. household detergents, fuels) are of better quality than conventional products	22	4.6

Table 6-2: Level of agreement with statements about renewable resources (representative telephone survey of 1,000 German citizens in 1996; data from Meinecke & Rosengarten 1996)

[111] Top two levels of agreement (7 or 6)
[112] 7.0 = full agreement; 1.0 no agreement at all

Population segment	Share in sample (%)	Key characteristics
Environmentally oriented	24	Large share of women and older (56-65), prefer the purchase of environmentally friendly products, very positive attitude towards renewable resources, but are of opinion that quality is lower and price must not be higher than of conventional products
Negatively oriented	23	Large share of men and young people (18-25), high formal education, low environmentally-oriented behaviour, negative attitude towards renewable resources, doubt benefit for agriculture
Cost oriented	22	Medium to high formal education, no environmentally oriented consumption patterns, strongly stress cost aspects of renewable resources
Critical-informed	16	Well-informed citizens with critical standpoint, in many respects rating equally the strengths and the problems related to renewable resources
Naïve-positive	15	highest share of women, elder people and pensioners, low to medium formal education, low knowledge about environmental protection and renewable resources, assume a better quality for products from renewable resources than for conventional products, but advocate for similar price levels of both product types.

Table 6-3: Key characteristics of population segments with different attitudes towards renewable resources

6.3.5 Insight gained from earlier studies

All of the five studies discussed above deal with the perception of the general public and are therefore fully within the scope of the BREW project. While the latest Eurobarometer survey (Gaskell et al. 2002) addresses enzymes, two studies deal with biodegradable plastics (Kassel Pilot Project and NatureWorks' study), one study (BMBF project) deals with industrial products with biodegradable plastics as a case study, while the fifth study (by the Renewable Resources Agency) is much broader in scope. Among the three studies dealing with biodegradable plastics,

- NatureWorks' study deals with PLA which fully complies with the scope of the BREW project (PLA is made by polymerization of the White Biotechnology product lactic acid).
- the BMBF project deals with Green Biotechnology for the supply of industrial products and feedstocks in general and with the case of biodegradable plastics in particular; while the technology scope hence differs from the BREW project, the resource base is identical (renewable resources).
- the Kassel project deals in general with biodegradable (compostable) plastics for packaging, including White Biotechnology products, bio-based products made without White Biotechnology (e.g., starch polymers) and biodegradable petrochemical products; the respondents in the Kassel project largely seem to equate the feature of biodegradability with the use of renewable feedstocks, thus making the outcome of this study more relevant for the BREW project.

Two sources, i.e. the Eurobarometer surveys (Gaskell et al. 2002; INRA/ECOSA 2000) and the BMBF study show that there is no general rejection of biotechnology if applied for

industrial products and if the benefits are perceived as being sufficiently high. This raises the question which factors lead to a positive understanding of the benefits. It is therefore an important finding that the BMBF study (see Figure 6-2) and the Kassel pilot project indicate a key role for environmental and health aspects in public perception. As shown by the BMBF study, these aspects obviously even overcompensate the generally bad image of Green Biotechnology: while Green Biotechnology is still suffering from the backlashes in the food sector, the overall assessment for its application to produce industrial products and feedstocks is clearly positive (see Figure 6-1). As explained in Chapter 5.2 there are good arguments that the risks for health and the environment are lower for White Biotechnology than for Green Biotechnology. Therefore, we can deduct from the BMBF study a clearly positive public perception also for White Biotechnology.

The finding about the outstanding importance of environmental and health aspects is crucial in view of the outcome of Section 6.2.4 according to which the number of factors contributing positively to the public perception of White Biotechnology is rather limited. There is hence strong indication that the notion of environmental and health benefits overcompensates the negative factors identified in Section 6.2.4. At the same time, the findings of the studies found are neither exhaustive nor precise. Previous results could only be used as *proxy* for the public attitude in Europe with regard to biotechnology and new bio-based materials. Given this limitation we conducted within the BREW project a survey taylored to White Biotechnology. This survey will be discussed in the next section.

6.4 The BREW survey

In Section 6.3 we showed that it is possible to draw conclusions about the public perception of White Biotechnology *only by deduction* from studies with somewhat different scope. Since no survey was available dedicated to White Biotechnology it was decided to conduct a survey of opinions and attitudes expressed by selected stakeholders in Europe. The goal was to set out a qualitative rating of the key determinants of public opinion. For reasons of comparison, it was chosen to include in the survey Green Biotechnology, conventional chemicals production and several other technologies next to White Biotechnology.

A questionnaire was developed (see Appendix 14) which was sent out to stakeholders who could be assumed to be informed about or involved in White Biotechnology, including:

- corporate officials,
- academics,
- researchers,
- government officials,
- non-governmental organisations (NGOs).

We chose to address stakeholders and not the general public mainly because a survey among laypersons would have required a much larger sample in order to ensure representativeness (this was not possible due to the limited resources available in the BREW project). As a further reason, stakeholders can be considered as primary actors of any public debate, considering also that:

- the products we are referring to are not foreseen to be end products available to final consumers but intermediary products;
- most European citizens are totally unaware of the possible implications of an industry that is just emerging. A survey of the public at large would therefore probably have yielded results that are less relevant and more difficult to interpret, while the evaluations provided by an expert sample group offer a more reliable and less volatile basis to assess the relative importance of the factors contributing to shape the public perception.

The questionnaire was sent out in November 2004 to a sample of about 300 stakeholders either by postal mail or electronic mail. The rate of responses, that continued to accrue until February 2005, was higher than expected (59 respondents, that is about 16%) considering the rather technical character of the survey.

Description of the respondents

The distribution of respondents is concentrated in Central Europe (Germany 31%, Belgium 20%, Netherlands 15%) and France (10%). The rest is scattered among Austria, the UK, Denmark, Switzerland, Ireland, Sweden, Finland, and Italy. Southern European countries are almost not represented and Northern European countries are underrepresented. Belgium is overrepresented due to the presence of international organisations in Brussels which were predominantly chosen as stakeholders to be addressed by the survey. Interesting conclusions could be certainly drawn from this pattern of distribution, however this would be outside the scope of the present analysis.

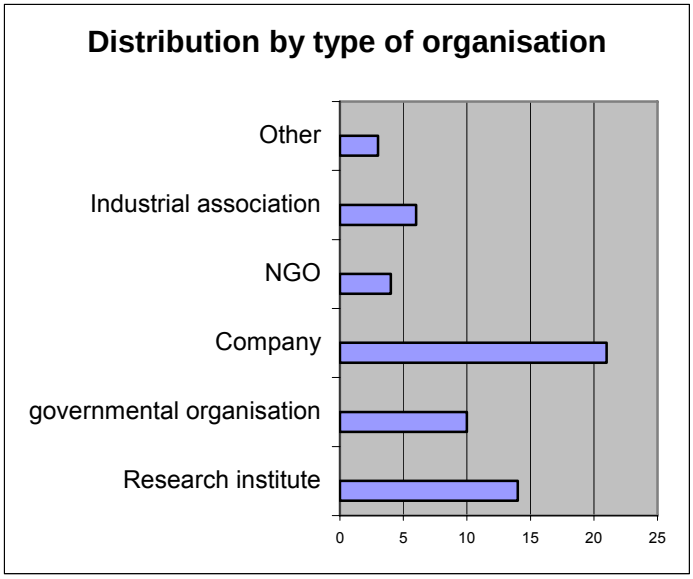

Figure 6-4: Distribution of respondents by type of organisation (in numbers of respondents)

As shown in Figure 6-4 the most numerous group is represented by company officials (36%), followed by researchers (24%) and public officials (17%). NGO members are very few; environmental and farmers' organisations are totally absent. Most respondents turned out to be actively involved in the field (58%), and the majority qualified as at least "knowledgeable" on the matter (64%) or even "expert" (19%). The sample is therefore representative for the public at large, however the results offer insights that help to identify some major trends of public perception because it can be expected that the stakeholders reacting to the questionnaire are or will be shaping public perception considerably.

Description of the questionnaire

The questionnaire (see Appendix A14) consists of a general part on bulk chemicals from renewable materials and a specific part on the case of polyhydroxyalkanoates.

The first part was aimed to assess the sustainability of the manufacturing of chemical bulk materials and chemical intermediates from renewable biomass compared with other possible options, i.e.

- food/feed production by conventional/organic agriculture
- energy production from fossil/renewable resources
- bulk and fine chemicals derived from fossil fuels.

The second part of the questionnaire focused on polyhydroxyalkanoates (PHA) which was chosen as an exemplary case to illustrate the various production options by means of

The four options

Option 1: The chemical industry produces PHA by bacterial fermentation in a reactor. Waste biomass (e.g. whey, hydrolysates of lignocellulosic waste, plant and animal wastes) is used as feedstock.

Option 2: The chemical industry produces PHA by bacterial fermentation in a reactor. The production organism is genetically modified to optimise its production characteristics. Agricultural crop plants (e.g. wheat or maize starch) which are only grown for this purpose are used as feedstock.

Option 3: Farmers produce PHA by growing special agricultural crop plants. The ability to synthesize PHAs has been conferred to these plants by genetic modification (= genetic engineering, gene technology).

Option 4: The chemical industry produces polymers functionally equivalent to PHA by chemical synthesis from fossil fuels.

The appraisal criteria

- Reduction of greenhouse gas emissions
- Reduction of fossil resources consumption
- Reduction of the economy's dependency on fossil resources
- Reduction of total energy requirements
- Decoupling economic performance and total energy requirements
- Need to demonstrate superiority for key environmental impacts (e.g. LCA)
- Sustainability in industrial production
- Sustainability in agriculture
- Supporting long-term international competitiveness of EU industry
- Contribution to the development of rural areas and to farmers wages
- Impact on agricultural land use
- Impact on local dimension (agricultural production and/or processing plants)
- Impact on centralised dimension (large-scale agricultural production and/or processing plants)
- Effects on preferences for sustainably produced goods and products
- Customers and consumers specific evaluation of the value for money and willingness to pay for it
- Need to allow customers/consumers to do an informed choice (labelling, standards, certificates).
- Social and/or regional distribution of benefits and costs/risks of this option (e. g. employment, income, environmental impacts, structural change) is fair
- Technical feasibility (with available state-of-the art knowledge and technologies)
- Need to introduce specific support schemes (e.g. policy priorities, regulations, RTD programmes, subsidies and taxes) for the realisation of this option
- Economic feasibility (production costs in an acceptable cost range)
- Need of incentives such as tax exemptions or subsidies to make the option economically attractive/viable
- Requirement of major adaptation processes along the value chain (new equipment, know-how, processes…)
- Need to pursue stakeholder involvement/consultations in decision making processes
- Favourable evaluation because it avoids the use of GMOs
- Undesired and unintended impacts of GMOs effectively prevented/managed
- Adventitious mixing of food and non-food crops of GMO and non-GMO products can be effectively prevented

Box 6-1: Overview of the four production options and of the appraisal criteria included in the BREW survey

biotechnology. In an analogous way, other chemical products could be produced. PHA are naturally occurring polymers synthesised by several living organisms, mainly bacteria, from biomass as substrate; they can replace certain plastics and also have unique properties for new applications. The questionnaire asked to assess four hypothetical production routes to PHA (see below), according to appraisal criteria chosen on the basis of the factors potentially triggering public response.

Results

The respondents were first asked to assess the level of sustainability of other technologies, in order to put the biotechnological production of bulk chemicals into perspective (see Figure 6-5). The most apparent finding is the widespread acknowledgement of the non-sustainability of producing chemicals and especially energy from fossil feedstock. The production of energy and bulk chemicals from biomass is mostly seen as potentially sustainable, "if improved". The scores given to the production of bulk chemicals from biomass are practically identical to energy production from biomass and energy production from renewable resources. No respondee assessed these technological options as "not sustainable" – differently from any other technology, even including organic agriculture and renewable energy.

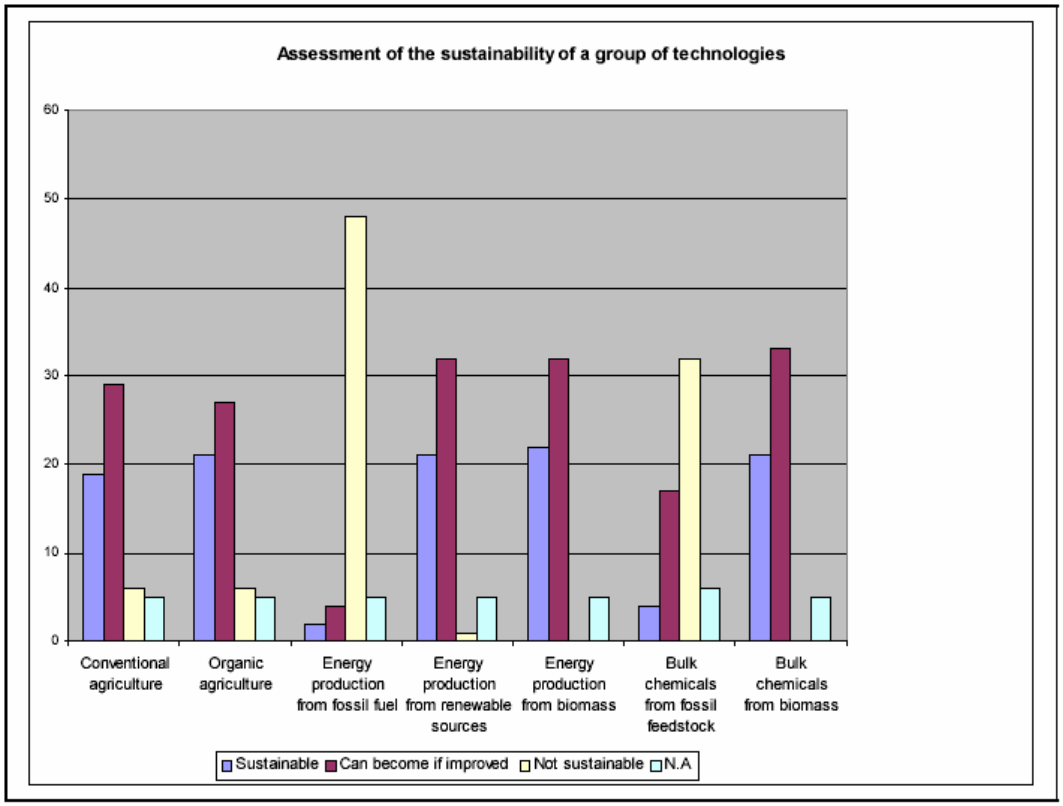

Figure 6-5: Expert assessment of the level of sustainability of various industrial activities (values on y-axis represent the number of responses)

The stakeholders were asked to evaluate to which extent a general shift from fossil feedstock to biomass in chemical production could contribute to sustainability if compared to other major technological developments. The respondents' attitude is optimistic, but cautious. Less than half of the sample (47%) consider such a development as one of "major importance", compared to 78% for the shift from conventional to renewable energy production.

A crucial point concerns the timing of an eventual shift from fossil-based to biomass-based production, addressed in the following question that compared bulk chemical production from biomass with production from fossil feedstock, in the present time and in the (unspecified) future. The stakeholders were not provided with any further information on the boundary

conditions (e.g. oil price) in the future. On the whole, the respondents' attitudes appear rather conservative: only 12% would immediately restructure bulk chemical production to use exclusively biomass as feedstock, and 49% wish to see such a shift in the future (Figure 6-6). It is remarkable that no respondent favours the idea of maintaining the chemical production entirely based on fossil fuel in the future. The preference for maintaining fossil feedstock as primary source is mainly justified with economic and technical feasibility reasons. The preference for biomass is rather explained by environmental, economic and geopolitical reasons. The geopolitical factor is not considered a key determinant for decisions about technological developments.

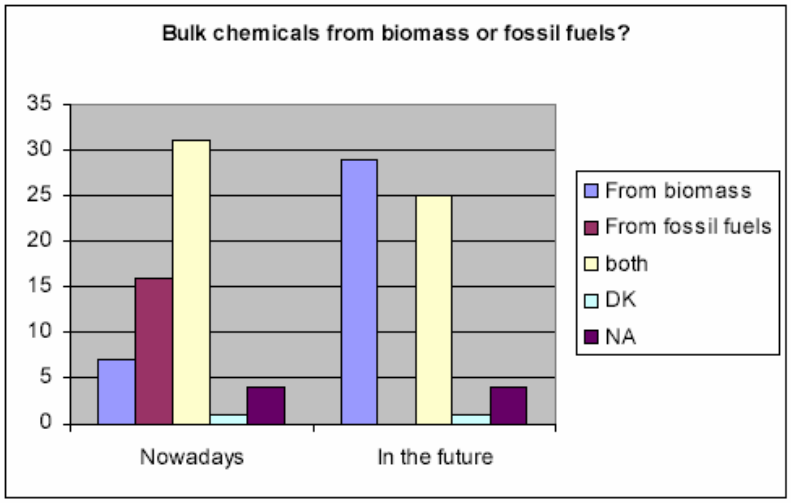

Figure 6-6: Expert assessment on the production of bulk chemicals from biomass and fossil feedstocks nowadays and in the future (values on y-axis represent the number of responses; legend: DK: "Don't know"; NA: Not available)

Biomass can be used to produce bulk chemicals as well as energy. Due to its limited availability biomass should be used in the most effective and efficient way. The majority of respondents does not seem to see the two uses as conflicting, maintaining that biomass should be used to produce both bulk chemicals and energy (Figure 6-7). Energy production is seen more as a priority in the present, while bulk chemicals production emerges as the priority in the future; all in all, however, this does not seem to be a critical point.

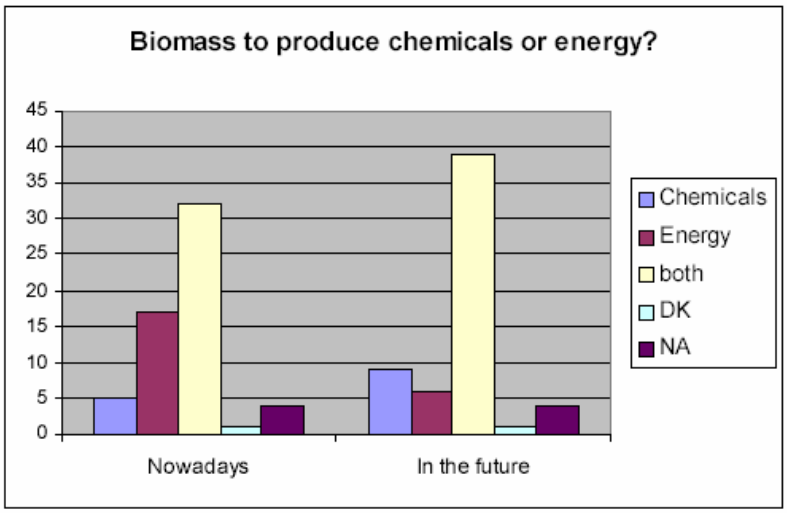

Figure 6-7: Expert assessment on the production of bulk chemicals from biomass and fossil feedstocks nowadays and in the future (values on y-axis represent the number of responses; legend: DK: "Don't know"; NA: Not available)

In future, White Biotechnology chemicals may be produced to a large extent outside Europe (e.g., in Latin America and Africa) due to more advantageous boundary conditions in these countries. This raises the question whether European governments should nevertheless support the European industry in order to help obtaining a leading role on global markets. When asked to reply to this question, 75% of respondents expressed the opinion that the European governments should support the industry even if the production occurs abroad. While this outcome may partly be the result of considerable share of the respondents having a pro-active attitude towards White Biotechnology and/or bio-based chemicals, the assessment result is significantly higher than for most other questions, indicating a broad support for domestic R&D on White Biotechnology regardless of the location of production.

A rather optimistic attitude is expressed by the respondents also concerning the possible environmental and health risks inherent in the use of biotechnology. In fact, 47% of the sample is "confident" that these risks can be successfully managed and 25% is even "sure" that such result can be achieved. Hence, nearly three quarters of the respondents do not see environmental and health risks as critical factor for biotechnology in general (the separate analysis for White Biotechnology and Green Biotechnology leads to the same conclusion, see below). If we assume this perception to be guiding for the future then the fears for possible risks are not likely to be a major obstacle to the development of this industry.

Concerning the development perspectives of the industry, a large share of the respondents (75%) believes that "the biotechnological production of bulk chemicals will become an important area for innovation and economic growth in the next 30 years" and 44% that "it will revitalise the petrochemical industry and contribute substantially to its international competitiveness".

The second part of the questionnaire aimed at exploring in detail the different implications of four technological options for bulk chemicals production (see also Box 6-1):

- Option A: Conventional chemical synthesis from fossil fuel
- Option B: Biotechnological production by naturally-occurring bacteria)

- Option C: Production by genetically modified bacteria
- Option D: Synthesis in genetically modified crops.

The latter option – i.e., the synthesis of bio-based chemicals in genetically modified crops - is outside the scope of White Biotechnology and is not studied within the BREW study; it was nevertheless included in the questionnaire for reasons of comparison. The part of the questionnaire devoted to the four options A to D was divided in 24 subquestions for specific aspects corresponding to single appraisal criteria; each criterion in turn was evaluated according to its perceived relevance (0 = undecided, 1= not important, 2 = somewhat important, 3 = very important). According to the weighing provided by the respondents, the first 10 criteria by importance are the following (the presentation of the results in grapical form can be found in Appendix A15):

1. Helps to achieve *climate protection* goals, because it contributes to the reduction of greenhouse gas emissions
2. Is likely to perform better than competing options regarding *key environmental impacts* such as total energy use, greenhouse gas emissions, etc. This superiority could be demonstrated through e.g. life cycle assessments.
3. Contributes to *saving fossil resources*.
4. Strengthens long-term *international competitiveness*, export position and innovation in the EU chemical industry.
5. Has *low production costs*.
6. Is *economically attractive* and viable without incentives such as tax exemptions or subsidies.
7. Reduces the country's *dependency on fossil resources* (e.g. oil imports, oil prices).
8. Helps to make industrial chemical production *more sustainable*.
9. Uses genetically modified organisms which could possibly lead to undesired and unintended impacts; however these can be effectively prevented and managed.
10. Serves customers' and consumers' preferences for goods and products that are produced by sustainable processes.

As an important finding, the environmental criteria (1, 2, 3, 8, 9, 10) turn out to be the most relevant according to the respondents' weighing, followed by economic criteria (4, 5, 6) and geopolitical criteria (7). The comparison of these criteria across the four options yields the following picture:

- In most cases, option A (conventional chemistry) was rated clearly inferior to the other three options.
- Regarding the three criteria which the stakeholders consider to be most important (see above: 1) Climate protection 2) Key environmental impacts and 3) Savings of fossil resources) the results are by and large similar for option B to D (Appendix A15). We find, however, a somewhat larger spread of replies for option D (especially with regard to climate protection and "Key environmental impacts"). Option B (naturally-occurring bacteria) is rated somewhat worse with regard to "key environmental impacts" than the GM options (C and D). While this is a somewhat amazing outcome, the differences are small and limited weight should be given to this result also because "key environmental impacts" were not defined in the questionniare.

- Economic aspects (rank 4 to 6) were covered in the questionnaire by the criteria "Low production costs", "economically viable without financial incentives" and "contribution to international competitiveness". Concerning the first two criteria ("Low production costs" and "economically viability") petrochemical production is considered to be clearly superior to the biotechnology options. Among the biotechnology options the reply pattern on production cost is quite diverging (virtually no reply "true"; relatively large shares of "false" and "undecided"; see Appendix A15) but option C (GM bacteria) clearly scores best (Appendix A15). This confirms the choice made in the BREW study (Chapter 3 and 4) to focus, *within* biotechnology, on *White* Biotechnology and to include also genetic modification of bacteria used in fermentation processes. The reason for the rather large divergence for the biotechnology options is probably that, at the beginning, economic viability is expected to be a challenge, hence explaining why a substantial share of respondents considers at least some financial support to be necessary (outcome on question on "economically viability without financial incentives", see Appendix A15). The positive view about the effects for international competitiveness (maximum replies for "true" and "partially true") may then be caused by the fact that the respondents have in mind the effects for the longer term. In other words, the survey results on economic criteria can be combined as follows: If the boundary conditions (including fiscal incentives) allow to master the economic challenge and to develop the biotechnology options then there will be clear benefits also for competitiveness.
- The results for option B to D are quite comparable concerning the effects for country's dependency on fossil resources (rank 7). All biotechnology options (B to C) score by far better than the conventional chemistry (option A). Comparable results across the biotechnology options are also found for the contribution to sustainability (rank 8), with a slight advantage for non-GM bacteria (Appendix A15).
- Concerning the manageability and preventability of unintended impacts of genetic enginering the respondents see hardly any difference between option C (GM bacteria) and option D (GM plants). This may be a somewhat unexpected result which, on the other hand, was already found by Voß et al. (2002; see Section 6.3.2).
- Regarding the aspect rated lowest, i.e. the customers' and consumers' preferences for sustainable products, all biotechnology options (B to D) score by far better than conventional chemical production (option A), thus confirming the outcome of earlier studies (see Section 6.3). Among the biotechnology options, option B (non-GM bacteria) scores best, followed by option C (GM-bacteria 10) and finally, option D (GM plants).

To summarize, the respondents consider White Biotechnology with GM bacteria (option C) as best choice among the biotechnology options with regard to production economics but this option still scores worse than petrochemical production. With regard to international competitiveness all biotechnology options score better than petrochemicals, indicating the promising potential for the future. The respondents do not see pronounced differences among the biotechnology options with regard to environmental impacts (including GHG emissions), risks and "sustainability". They do, however, acknowledge that consumers and customers prefer non-GM products. This overall result is confirmed by the replies to the request for a "ranking of the technology options according to personal assessment" which is shown in Figure 6-8.

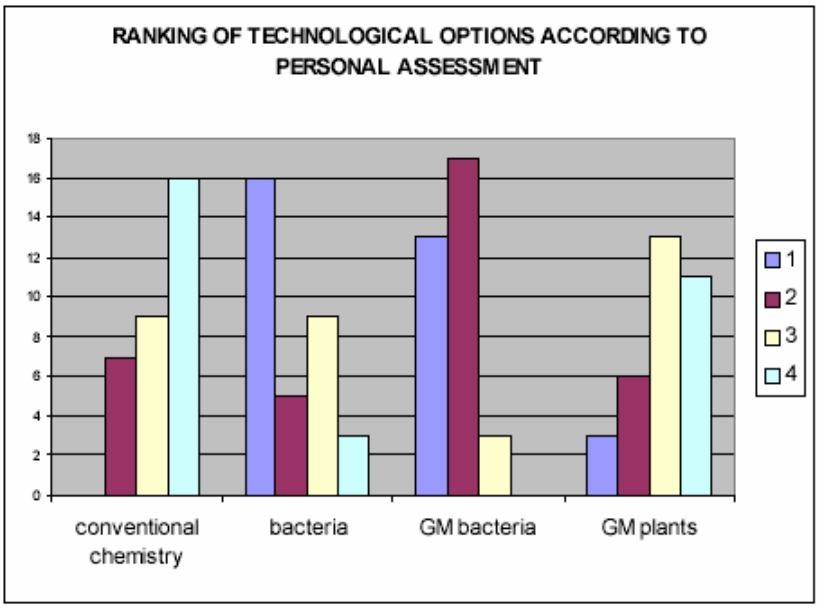

Figure 6-8: Ranking of technological options according to personal assessment (values on y-axis represent the number of responses; legend: 1 =most favoured option; 4 =least favoured option)

Disaggregated analysis

As explained at the beginning of this section (Figure 6-4) most of the respondents are actively involved in the field, which is likely to cause a positive bias of the results. In order to separate the "insider" views from the views of the rest of the sample, considered as a more realistic "proxy" of the general public, we split the sample into two components: "industry" (N = 21), including representatives of industrial companies, and "other respondents" (N = 38). The separate analysis indeed shows considerable differences between the two groups of respondents (see Figure 6-9): A more conservative attitude is expressed by the "industry" group toward the idea of shifting from fossil to biomass feedstock in chemical production (48% would maintain fossil fuel in the present compared to 16% for the "others" group), though the difference seems to even out as far as "the future" is concerned. No significant differences are found concerning the respondents' attitudes to risk inherent in biotechnological production. Optimism appears overwhelming in both groups also concerning the development perspectives of the new technology in terms of innovation and economic growth.

Where the positions of the two groups appear very distant is when it comes to weighing the criteria used to appraise the four technological options for chemicals production. Here the different value sets clearly emerge as shown by the following comparison of the (implicit) rankings of the criteria made by the two groups: The industry group attaches much more importance to economic and legal criteria while for the non-industry respondents, the environmental criteria play a dominant role and considerable attention is given to aspects related to agriculture and farmers' conditions that are totally ignored by the former group. Finally, the geopolitical factor (dependency on oil imports) seems not to be relevant for the industry group, while it ranks high for the rest of the sample. The ranking of the four technological options according to personal assessment for bulk chemicals production is

significantly different for the two groups (Figure 6-9; compare Figure 6-8 for the total of *all* respondents):

- The "industry group" prioritizes the options as follows (most desirable option is mentioned first): first GM bacteria, second conventional chemistry, then naturally occurring bacteria and finally GM plants.
- The non-industry group prefers naturally occurring bacteria, then GM bacteria, GM plants and conventional chemistry.

However, considering the ranking as a whole, the difference between the two groups is not so sharp and should not be overinterpreted.

The separate analysis for industry and non-industry respondents was also useful to assess to which extent the bias inherent in the composition of the sample might invalidate the results of the survey. In fact, splitting the sample helped to distinguish between opinions that are more directly related to an "insider" position and those that could be seen as reflecting the views of the general public, though articulated by "experts". Most outcomes of the survey received further confirmation as the results for the entire sample were not reversed by the "non-industry" respondents.

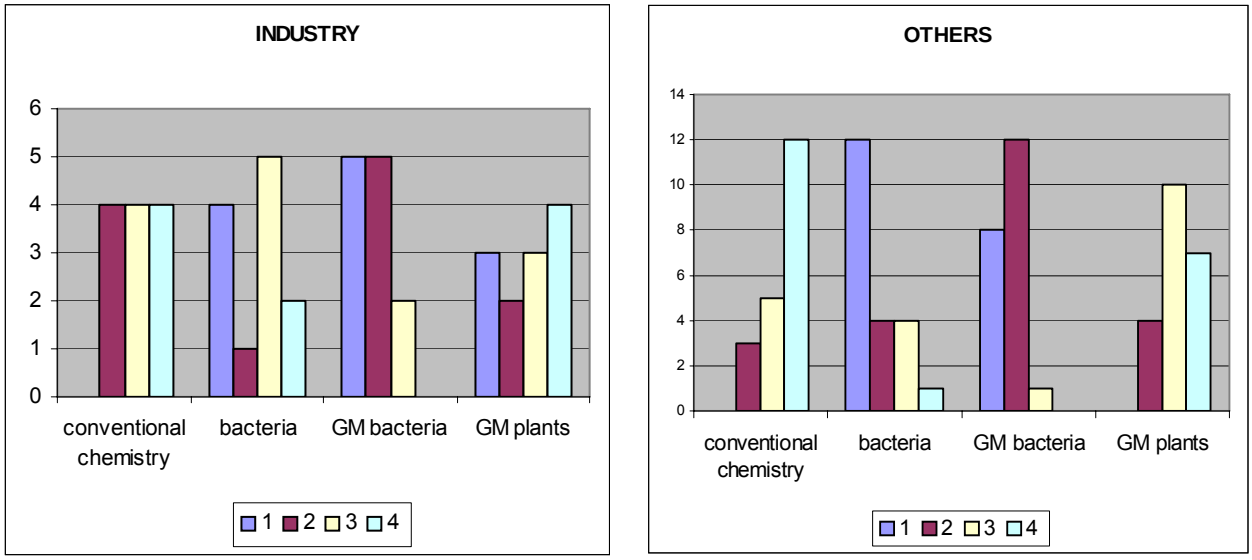

Figure 6-9: Ranking of technological options according to personal assessment by i) industry representatives and ii) all other respondents (values on y-axis represent the number of responses; legend: 1 =most favoured option; 4 =least favoured option)

6.5 Conclusions

In this section we compare the outcome of the BREW survey with the insight gained from the studies (Section 6.3), with the objective of drawing overall conclusions. We do not base the conclusions exclusively on the BREW survey due to the fact that survey was conducted among stakeholders with a strong representation of experts from the chemical industry. This introduces the risk of a bias. This bias seems to be limited to very limited as the separate analysis for experts from industry and non-industry experts shows. Among the studies taken into account, most references will be made to the BMBF project and to the Kassel Pilot Project because most detailed information was available from these sources. However, also the other studies taken into account support the reasoning below very well.

Comparing the level of sustainability across technologies, the BREW survey shows that White Biotechnology products reach **practically the same scores as renewable energy**, among them bioenergy.[113] Apart from Figure 6-5 this becomes visible also from the BREW survey respondents' view that biomass use for the production of chemicals and for energy should be pursued simultaneously (Figure 6-7). These insights gained from the BREW survey are supported by the Kassel survey according to which approximately 90% of the respondents agree that biodegradable polymers will have a similiar relevance as future wind and solar energy. This finding is very important in view of the generally very positive public perception of renewable energy.

The main reason for this clearly positive overall view of bio-based chemicals is the understanding of **substantial environmental benefits**: The respondents of the BREW survey rate the "key environmental impacts", fossil resource savings and climate protection benefits to be much higher for chemicals produced from biofeedstocks by means of biotechnology as compared to conventional petrochemical polymers. This positive assessment concerns both organic bulk chemicals produced by White Biotechnology (fermentation and enzymatic conversion) and by Green Biotechnology in agricultural crops (with rather little difference between the two for the three criteria just stated). This is fully supported by the BMBF study (for Green Biotechnology chemicals) which identified environmental aspects as the most important determining factor for the respondents' overall assessment of non-food products. Also the Kassel project indicates a strong correlation between environmental benefits and general acceptance (with the latter being reflected by a high degree of agreement with the substitution of biodegradable polymers for concentional plastics). The same is true according to Eurobarometer (Gaskell et al. 2002) for enzymes produced by genetically modified enzymes.

The expectation of substantial environmental benefits is dominated by the positive connotation made between bio-based chemicals and the reduction in fossil energy use and greenhouse gas emissions but it also accounts for other aspects, in particular risks to the environment (biodiversity) and to human health. These risks to environment and health do not seem to be of major importance for public perception: According to the BREW survey nearly three quarters of the respondents (both industry experts and non-industry respondents) are confident or sure that risks can be successfully managed. This is in line with the insight

[113] This statement is valid for the entire sample. The subgroup of industry experts expects bulk chemicals from fossil feedstocks to score better in termes of sustainability than renewable energy, while the opposite is true for non-industry respondents.

gained from Eurobarometer and from the BMBF project according to which no general rejection of biotechnology is to be expected. The BREW survey clearly shows that

- White Biotechnology (regardless whether *with* or *without* genetic engineering) is clearly favoured over Green Biotechnology (Figure 6-8)
- that non-industry respondents favour non-gene modified microorganisms over gene modified microorganisms (Figure 6-9).

We conclude firstly that the **overall level of acceptance for the biotechnological production of industrial products is rather high** but secondly that **important differences exist among the biotechnological production options which should be taken seriously.**

Given the - essentially unanimous - high importance attributed to environmental benefits, the ranking among all major packaging materials (among them plastics, glass, metal and paper) according to the Kassel project provides very interesting insights: according to this ranking biodegradable polymers are rated most favourably while conventional polymers take the lowest position. This indicates that the production of chemicals from biofeedstocks instead of fossil fuels **contributes clearly positively to the chemical industry's image in the public.**

Given the higher price level of most bio-based chemicals today, **economic considerations** are nowadays not a driver for bio-based chemicals. There is, however, some willingness to compensate for this disadvantage since, according to the Kassel project and the survey commissioned by NatureWorks, consumers are willing to pay a surcharge for bio-based products. As shown by the BREW survey also stakeholders questioned are aware of the disadvantages in production costs compared to conventional chemicals (see Appendix 15; this is fully supported by Chapter 3 and 4 of the BREW study). The stakeholders seem to see this as a transitional phase, as an "investment into the future", which pays back in the form of improved international competitiveness. This is consistent also with the positive attitude towards policies and measures in the BREW survey (in the form of "fiscal incentives", see Appendix 15) and according to the Kassel Pilot Project ("laws for saving oil and strengthening climate protection").

Socio-economic aspects in the form of employment effects are mentioned in the BMBF project but are not perceived as an important driver according to the other surveys (hardly addressed or not mentioned at all). Also **geopolitical factors** are not ranked as a priority among the factors influencing public perception and acceptance of White Biotechnology even though there do seem to be differences across the stakeholders. However, in the BREW survey, the reduction of dependency on oil imports is placed by the respondents among the 10 most important criteria used to appraise alternative technological options. The importance of this aspect is seen as relatively less relevant at present, but increasing in the future. Even potentially controversial issues linked to agricultural production of renewable resources are perceived as relatively irrelevant, as confirmed by the low response rate of farmers' organisations in the BREW survey and the fact that monocultures, fertilizer use and GMO are mentioned in the Kassel project but obviously do not influence significantly the overall perception.

As important caveat, it should be considered that the BREW survey and the five studies discussed no not address or hardly account for a number of aspects, with the most important being:

- hardly any of the sources taken into account can claim being representative for the *perception of White Biotechnology by the general public in Europe* because this has so far not been studied as such; the conclusions are therefore based on studies and samples which are biassed towards experts (especially in the BREW survey but also in the BMBF project), which differ with regard to the subject matter and which often have a smaller geographical scope (differences in public perception across European countries have hence not been taken into account while they may be important as some of the Eurobarometer results indicate).
- a whole range of issues concerning the effect of the introduction of extensive biomass crops in the EU agriculture, namely changes in land use patterns, impact on landscapes, alternative uses of biomass, economic implications for farmers and rural economies;
- the acceptance of the actual development of biomass plants at the local level by local communities (importance of appropriate siting, trust in local authorities and the industry);
- the public perception of socio-economic benefits accruing to the EU citizens following the development of industrial biotechnology (for example in terms of job creation, price of final products);
- the impact on public perception of eventual incidents at production plants, especially in case of accidental release of GM organisms; and
- the change of public perception over time over time as a consequence of improved scientific insight (disseminated by the media) and as a result of the gradual transition from niche production with a "small-is-beautiful" bonus to a full-scale, internationally operating industry.

Given the early stage and the complexity of this new technology, these omissions were inevitable. However, based on the available insight it seems probable that the *most relevant* aspects for today and for the short to medium term are adequately addressed.

An important finding of this chapter is that a **basically positive attitude** toward the development of White Biotechnology for bulk chemicals can be expected due to the prospects of large environmental benefits as a consequence of the use of renewable raw materials. This conclusion is based on studies and surveys with a somewhat diverse scope while more certainty can only be ensured by means of a study dedicated to public perception. This limitation should be kept in mind also for the following conclusions.

We further conclude that **technophobicity**, often quoted as obstacle for other technologies, **does not seem to be a critical issue for White Biotechnology**. Along similar lines, the **possibility to improve substantially the image of the chemical industry** endorses activities in this area. White Biotechnology can probably rely on strong public endorsement provided that its image of ecologically-compatible alternatives to conventional chemical production is maintained. There is also indication that the public is rather in favour of (or at least not rejecting) **supportive policies and measures**. The fact that the trust in White Biotechnology is based on the promise of clearly lower environmental impacts implies, however, that this technology **must live up to this expectation** with all its facets, i.e. including not only energy use and greenhouse gas emissions but also all other major environmental impacts such as risks related to genetically modified organisms. **Transparency** about the status and prospects in these matters is very likely to be critical for a continued positive perception.

7. Summary and Conclusions

White Biotechnology, the use of biotechnology in industrial production, is gaining momentum in the EU. It is generally expected that White Biotechnology can contribute to mastering the following societal challenges:

- Contributing to the international competitiveness of the EU chemical industry through process and product innovation and technological leadership,
- Saving resources and reducing environmental impacts of chemical production through "greening" of the chemical industry,
- Exploiting biomass as feedstock for industrial and energy production.

While biotechnology has already taken shape in the production of pharmaceuticals, fine chemicals and speciality chemicals and is expected to expand considerably in these sectors in the short to medium term, there is substantial uncertainty about when, how and to which extent biotechnology will also play a role in the production of *bulk* chemicals. It was the aim of the BREW project to address these questions in a comprehensive manner, taking into account scientific-technical developments as well as economic aspects, environmental impacts and societal drivers. While White Biotechnology comprises both renewable (biomass-based) and non-renewable (fossil) feedstocks for the production of industrial commodities, the BREW project is restricted to products based on renewable resources. This choice has been made because of the larger potential to reduce substantially the environmental impacts and because renewable feedstocks are the most common choice in White Biotechnology.

The production of bulk chemicals from biomass differs in many challenging aspects from the biotechnological production of fine and specialty chemicals. For example, the production volumes are larger, the product prices are rather low, process innovation is more important than product innovation and there is strong competition with well-established, optimised chemical processes. Assessing the potentials of biotechnology in the production of bulk chemicals from biomass is highly uncertain because it is a long-term development with gradual implementation until 2050. This process is expected to be driven by the progressive depletion of fossil resources, an increasing competitiveness of renewable feedstocks and increasing environmental pressure. In addition, it implies a paradigm shift in the underlying chemistry: from the conversion of hydrocarbons to the conversion of carbohydrates, thus requiring fundamentally different chemical reactions and processes.

In this report we provided an overview of the technical possibilities of White Biotechnology (Chapter 2), we analysed the environmental and the economic aspects on a product-by-product basis (Chapter 3) and in scenarios (Chapter 4), we assessed the conventional and non-conventional risks (Chapter 5) and we studied public and stakeholder perception (Chapter 6). The *main findings* are summarized below in Section 7.1.1 to 7.1.4. If, based on these and other insights, the European Union arrives at the conclusion that White Biotechnology is a key technology field for the future, it is strongly recommended to **develop an integrated White Biotechnology strategy**. Such a strategy should address four basic requirements which we derive in the *final conclusions* (Section 7.2).

7.1 Summary

7.1.1 Emerging White Biotechnology products

Based on a literature survey we developed an overview of chemicals which can be produced by White Biotechnology. In a first screen, an extensive list of possible bio-based chemicals was compiled (see Figure 2-1, Tables 2-28, 2-29). It was found that several bio-based chemicals are produced on bulk scale[114] already today (Table 2-41), which is in contrast to the wide-spread notion that biotechnology is not suitable for bulk chemical production. However, most of the products listed in Table 2-41 only account for a minor amount of total chemical production; and the main use of the chemicals produced in amounts of more than 200 kt/year is in the food, feed and fuel sector, but not for chemical purposes.

The extensive list of possible bio-based chemicals (see Figure 2-1 and Table 2-28 and 2-29) was subjected to further assessment by a product-tree approach as described in the introduction to Chapter 2, in order to identify building blocks of key importance for a possible future transition from petrochemicals to bio-based bulk chemicals. This led to the selection of 19 building blocks plus derivatives of natural fats and oils as representatives for complex products and finally genetically modified crop plants. These products have been discussed in detail in Chapter 2.1 to 2.7. For each product, the key features of production and use are discussed (e.g., biotechnological options, level of maturity, commercial status, world-wide production volume, challenges and drivers). The exclusion of products for which biotechnological processes are not necessarily involved and further exclusions and additions based on the evaluation of the partners of the BREW team led to a selection of 21 bulk products as top candidates for White Biotechnology (see Table 2-42; these products are analysed in-depth in Chapter 3 and 4). There is some correspondence between these selected products and those identified by Werpy and Petersen (2004; see first column from the right and footnote to Table 2-42). The difference between the two product lists is mainly caused by different terms of reference. Within the BREW project, the aim was to identify *bulk* chemicals produced from biofeedstocks by means of biotechnology, whereas Werpy's and Petersen's (2004) objective was to identify top value added chemicals from biomass sugars within the concept of an integrated biorefinery which produces fuels, high-value chemicals, materials and power. Moreover, the difference between the two assessments reflects the rather broad range of possible outcomes as a consequence of incomplete and uncertain data.

The selected building blocks can be distinguished according to the prevailing strategy for their market entry (termed "strategic fit criteria" by Werpy, Petersen 2004). We distinguish four strategies the first two of which play a key role in decision making. These **two key strategies** are:

- *Direct substitution of a bulk petrochemical.* This strategy implies that a bulk chemical which is presently produced from petrochemical resources would be substituted by an identical substance, produced from biomass with the help of biotechnology. Advantages of this strategy are that the markets for these products already exist but on the other hand, the bio-based products have the disadvantage to have to compete on a cost basis against optimised and often depreciated plants.

[114] Bulk scale was defined here as an annual production volume of at least 20-50 kt worldwide.

- *Functional competition of bio-based bulk chemicals with fossil-based ones*. When making the transition from petrochemical to bio-based production, it will not always be necessary or possible to provide the same product. Rather, a comparable or even superior functionality could be provided. Cost-competition with petrochemicals becomes less important if a new or improved functionality can be provided.

Some of the selected 21 White Biotechnology chemicals belong to *both categories*. For example, PTT made with bio-based PDO can be substituted for PTT made with petrochemically based PDO (direct substitution); but PTT made with bio-based PDO can also replace PET or nylon polymer, depending on the application (functional substitution). When categorizing the 21 chemicals according to the *stage of development* we find that all stages are represented (idea, feasibility, pilot stage and commercialised). Commercialised processes for building block production presently rely on glucose, sucrose or starch as *feedstock*, while future processes could make use of lignocellulosic feedstocks which are converted to fermentable sugars such as glucose, xylose and arabinose. Due to strongly increasing availability of glycerol as by-product of biodiesel production, glycerol may be increasingly used as fermentation feedstock. Finally, instead of using biofeedstocks derived from conventional agricultural crops, White Biotechnology could also make use of feedstocks derived from genetically modified crops (Green Biotechnology) if these have better properties, are less expensive or have other advantages, e.g in cultivation. The use of genetically modified crops is, however, no prerequisite for White Biotechnology.

We conclude from the above and the overviews of the individual products (see Chapter 2.1 to 2.7) that **White Biotechnology offers numerous opportunities for the manufacture of new and existing organic bulk chemicals** from a variety of feedstocks and that, given the early stage of development for most products and processes, **very substantial progress can be expected** for the future. **According to our assessment, the large-scale manufacture of White Biotechnology chemicals is technologically challenging but there is a wide range of interesting options and it does seem feasible for the longer term.**

7.1.2 Environment and economics

While, from a (bio-)chemical and a technological point of view, the opportunities are interesting and promising, the attractiveness for industry and policy depends to a very large extent on whether White Biotechnology products offer advantages in economic and in environmental terms. So far, quantitative analyses on the environmental impacts and the economic aspects related to bio-based bulk chemicals produced by White Biotechnology are scarce and fragmented. Published information is often not comparable due to different assumptions and boundary conditions. As a general difficulty, data availability is very limited because only few processes are already implemented on industrial scale and in most cases, data are kept confidential because they represent sensitive information.

It is a key goal of the BREW study to close this gap of knowledge in the public domain. The environmental and economic assessment represents the core of this report (Chapter 3 and 4). The environmental and economic assessment was performed at two levels:

- Firstly, the options were analyzed on a product-by-product basis with 1 mass unit (1 tonne) of product as reference. These analyses were performed for different prices for fermentable sugar but only one oil price (US$ 25/barrel crude oil; for natural gas, a price

of 4 €/GJ was assumed for final users in the chemical sector; Appendix A3-2). The product-by-product analysis has been discussed in Chapter 3.4.

- Secondly, the environmental and economic assessment has been conducted in the form of scenario analysis which takes into account the different market potential of the White Biotechnology products in view of their product properties and the economic boundary conditions. Here, both different sugar prices and different oil and gas prices are considered. The scenario analysis has been discussed in Chapter 4.

In both cases – the product-by-product analysis and the scenario analysis – petrochemical products were used as benchmark for the comparison. Problems related to the lack of data were overcome by the support of the BREW project partners who provided confidential information for the purpose of this project. As a further solution to the problem, we developed a White Biotechnology assessment tool – called **BREWtool**. This tool includes a **Generic Approach** for the assessment of White Biotechnology processes. This enabled us

- to solve the problem of missing or incomplete data
- to perform assessments based on uniform assumptions and boundary conditions, thus allowing true technology comparisons
- to broaden our knowledge base by analysing a substantive number of products/processes (21 in total), most of them with several process alternatives
- to conduct *ex-ante* assessments of White Biotechnology processes and products, which is needed in strategic R&D in industry, academia and in policy.

Regarding environmental performance, we studied only non-renewable energy use (NREU), greenhouse gas emissions (GHG) and land use. We limited ourselves to these aspects because the extension to other indicators would require more detailed process design studies or even measured data from existing large-scale facilities; none of which are available at this stage. Risks related to human health and the environment have been analyzed separately (Chapter 5) and are discussed later on (Section 7.4).

The **findings** of the product-by-product analysis and of the scenario analysis with regard to the **environmental aspects** of White Biotechnology can be summarized as follows (see Chapter 3.4 and Chapter 4):

- When summarizing the results in general, a distinction must be made between enzymatic processes and fermentation processes. In many cases, enzymatic processes may offer limited or even no improvement potential for non-renewable energy use (NREU) and greenhouse gas (GHG) emissions compared to conventional catalytic processes (see Section 3.4.5). The reason is that the conventional catalytic processes operate at quite mild conditions and that the energy use of these conventional processes is already very low. If toxicity, waste and product properties are taken into account, enzymatic processes may be clearly advantageous; however, these aspects were not analyzed in detail in this study.
- On the other hand it is also very likely that enzymatic conversions will play a key role in commercial future processes for the conversion of lignocellulosics to fermentable sugar. If process features and the economics allow to implement this type of process at large scale, it would offer major advantages in terms of non-renewable energy use and GHG emissions (see Section 3.4 and 4). In this sense, enzymatic processes are crucial for a

future chemical industry applying White Biotechnology to produce bio-based bulk chemicals.

- In contrast to enzymatic processes for which the picture is diverse, *nearly all* fermentation processes studied offer substantial reductions in NREU and GHG emissions compared to the petrochemical process already today and even more so, in the future. The following findings on environmental aspects are therefore limited to fermentation processes.
- If sugar based on maize starch is used as feedstock for fermentation, NREU savings seem possible already today for all products studied except for adipic acid and acetic acid, for which process optimization could change the picture. Compared to petrochemicals, the potential average cradle-to-factory gate NREU savings (arithmetic mean without adipic acid and acetic acid[115]) of all the products studied is 30% with current technology (TODAY) and it increases to 50% if R&D over the next 2-3 decades is successful. Reductions in GHG emissions are in a similar order of magnitude (this applies also for the other feedstocks, see below).
- The use of lignocellulosic feedstocks in fermentation offers for the FUTURE average cradle-to-factory gate NREU savings of 75% compared to the production of petrochemicals nowadays. Compared to the use of maize starch (FUTURE), the use of lignocellulosic feedstocks is hence expected to reduce NREU emissions by at least additional 20% in the FUTURE provided that the conversion of lignocellulose to fermentable sugars (C_5 and C_6 mixtures) can be successfully developed and if the conversion of this mixture of fermentable sugars to target chemicals can be realized with the same efficiency as foreseen for products based on maize starch (values again exclude adipic acid).
- Finally, by using fermentable sugar from sugar cane, cradle-to-factory gate NREU can be reduced relative to the current production of petrochemicals by around 80% for TODAY's technology and the savings reach nearly 100% in the FUTURE.
- Absolute NREU savings for Europe (EU-25) depend on the scenario chosen because this determines the extent of market diffusion of White Biotechnology chemicals. We distinguish here between a scenario LOW with rather unfavourable conditions for bio-based chemicals (oil price up to 30 US$/barrel; sugar price of up to 400 €/t; 0% p.a physical growth in the chemical sector), a scenario MEDIUM (up to 66 US$/barrel, up to 200 € /t sugar and 1.5% p.a. physical growth of organic chemicals) and a scenario HIGH (up to 83 US$/barrel, approx. 70 €/t sugar and 3.0% p.a. physical growth of chemicals). Therefore, in the scenario LOW in 2050, about **7%-10%** of the energy demand for the production of the selected chemicals studied are saved, while in the scenarios MEDIUM and HIGH this percentage is about **20%-30%** and **39%-67%**, respectively (lower values for starch, higher values for lignocellulosics; see Section 4.5.2 and Appendix 11-13).
- Instead of comparing the savings of energy and GHG emissions to the *production of the selected chemicals*, they can also be compared to the *total production of all organic chemicals*. For clarification: in our study we regard only a selection of possible bio-based chemicals and, thus, analyse only a fraction of the petrochemical market today: while in 2000 about 70 million tonnes of petrochemicals were produced in Europe (see Section 4.4.4), about 31 million tonnes (or about 50%) are within the scope of this analysis. Even

[115] Adipic acid and acetic acid were excluded because they both do not offer cradle-to-factory gate NREU savings TODAY. However, very substantial improvement potentials were identified for the FUTURE, with cradle-to-factory gate NREU saving potentials of 40% for adipic acid; for acetic acid it depends on the feasibility of the individual process designs studied whether this product will become in future an interesting candidate (up to 30% savings) or not (up to 40% higher NREU use in spite of process improvements).

though White Biotechnology chemicals might replace some of the excluded petrochemicals, we assume here that White Biotechnology does not offer any significant NREU and GHG savings in addition to those studied in Chapter 3 and included among the selected chemicals (Table 4-4). While this is a conservative assumption, it seems justified because i) the most promising White Biotechnology chemicals currently discussed have been taken into account, ii) the assumptions made in the Generic Approach represent upper limits (horizon values; see Section 3.1.1) and iii) no technological progress has been assumed for the production of petrochemicals (assuming technological progress for petrochemicals would reduce the saving potentials calculated for White Biotechnology chemicals).

Dividing the NREU savings from White Biotechnology products by the NREU for the *total production of all organic chemicals* gives saving percentages for 2050 of **3-5%** in the LOW scenario, **9-14**% in the MEDIUM scenario and **18-32**% in the HIGH scenario (within each range, the lower value is for starch and the higher value for lignocellulosics; see Section 4.5.2 and for detailed results by feedstock and year see Appendix A13). The lower saving percentages compared to those given in the preceding paragraph reflect the fact that the *total production of selected organic chemicals* is for all years around half of the *total production of all organic chemicals* (e.g., approx. 31 Mt versus 70 Mt in 2000).

- Today, the NREU (including primary energy equivalents of power production) of the total chemical industry in OECD Europe represents around 9.5% of the total energy (total primary energy supply) in all OECD Europe countries. Under the assumption that the importance of energy use in the chemical sector will not change decisively in the decades to come we can multiply this share (9.5%) with the saving percentages just discussed (between 3% and 32%). We hence estimate that White Biotechnology chemicals allow to save in 2050 0.3% to 3.0% of the non-renewable energy use (NREU) of the entire economy (the range covers all three scenarios for starch and for lignocellulosics; Section 4.6.2).
- While the findings discussed so far refer to cradle-to-factory gate NREU, the results for the various options studied for the system cradle-to-grave are in a very similar range. The same is true for cradle-to-grave GHG emissions.
- Due to the diversity of the fermentation processes studied and the differences in product properties across the chemicals studied (e.g., polarity, volatility, propensity to crystallize etc.) it is not possible to make general statements about the saving potentials by category of chemical compounds (e.g., carboxylic acid, alcohol etc.). Individual analyses are hence indispensible.
- The expected improvement potentials for NREU and GHG between TODAY's technology status and the FUTURE are enabled by both larger productivities and broth concentrations in the fermentation step and also by clearly improved product separation and purification schemes (see Table 3-2). Compared to the clear improvements in productivities and broth concentrations, the expected increase in product yield between TODAY and the FUTURE is relatively limited.
- As a consequence of this relatively limited increase in product yield between TODAY and the FUTURE (see Table 3-2), the expected contribution of future R&D in White Biotechnology to higher land use efficiency (ha/t product) is also relatively limited. This statement refers only to the conversion of fermentable sugar to target chemicals, while the successful conversion of lignocellulosics to fermentable sugar would probably lead to a

step change, with land savings in the order of 60% compared to maize starch-based products.[116]

- The total land use for bio-based chemical production is relatively low in most scenarios. If starch is used as basis for fermentable sugar, the total land use ranges from 1.0 to 38.2 million ha in the three scenarios. If lignocellulose is used as biofeedstock, only 0.4 to 15.6 million ha are needed. For comparison, the agricultural area in the EU-25 was about 179 million ha in 2002 (FAO 2005). Land requirements are hence not likely to become a critical issue in the next few decades (Section 4.5.2).
- In order to understand the relationship between saved NREU (compared to the production of petrochemicals) and land requirements - i.e. the ratio of the two parameters - can be determined. This understanding can help to maximize NREU savings for a given amount of land or, vice versa, to minimize land use if a certain amount of NREU is supposed to be saved. Another important application for policy makers is the comparative analysis with bioenergy in order to understand which of the two options – bioenergy or bio-based chemicals – offers larger NREU saving potentials per hectare of agricultural land. White Biotechnology chemicals score clearly better than liquid biofuels (ethanol) with regard to the non-renewable energy savings per unit of agricultural land used. The White Biotechnology chemicals are, however, comparable to the non-renewable energy savings that can be achieved by co-combustion of biomass in coal-fired power plants: For *starch*-based chemicals the average savings are 110 ± 30 GJ/ha which is similar to co-combustion of poplar with 115 GJ/ha.
- While this study focusses on NREU, GHG emissions and land use, other environmental impacts are dealt with in qualitative terms, wherever possible. One important finding is that high salt loads in the wastewater of fermentation processes can - and should - be avoided. The findings from the analysis on risks are discussed below (Section 7.3).

The **findings** of the product-by-product analysis and of the scenario analysis with regard to the **economics** of White Biotechnology can be summarized as follows (see Section 3.4 and Chapter 4):

- As for environmental aspects, a distinction must be made between enzymatic processes and fermentation processes when summarizing the results of the economic analyses: in conjunction with innovative separation processes, enzymatic processes are expected to enable substantial cost reductions rather soon while, for most fermentation processes, economic viability is a more challenging goal for production facilities located in Europe. The following finding concerns enzymatic processes while the remaining points on economics concern fermentation processes.
- In order to make enzymatic processes widely economically viable (see Section 3.4.5), enzyme costs for small-scale processes (around 10 kt p.a.) would need to drop to around 100 €/kg, while enzyme costs for larger scale processes (around 100 kt p.a.) would need to drop to a few tens of Euros per kg of enzyme; major cost reductions of this magnitude seem feasible.

[116] The saving potential for land use stated here refers to fermentable sugar from lignocellulosic waste streams (maize stover) which is the default case of our calculations with BREWtool (see Section 3.4.1). Other approaches would lead to other results.
The use of fermentable sugar from sugar cane does not offer any saving potential for land use compared to maize starch (based on arithmetic mean of specific land use for all products studied).

- Based on our limited sample of fermentation products (see Section 3.4.4) we conclude that substantially more products become economically viable if sugar prices are reduced from 400 €/t to the globally lowest level of 70 €/t (as currently found in Brazil); a sugar price reduction from 400 €/t to 200 €/t already makes a substantial number of products economically viable (Table 3-10).
- Around two times as many fermentation products become economically viable if, for a given sugar price, optimal technology is assumed instead of the current state-of-the art (this statement is based on the small sample of products we studied; see Table 3-10).
- As a consequence, the opportunities for fermentation products improve tremendously under the condition of low sugar prices in combination with highly efficient technology (as it may become available in the long term future) as opposed to the current situation in Europe with high fermentable sugar prices and today's state of the art technologies (Table 3-10).
- The market potentials for fermentation products differ considerably for the three scenarios (LOW, MEDIUM and HIGH; see definitions above). While in the scenario LOW in 2050 only about 5 million tonnes of bio-based chemicals are produced, the respective values for the MEDIUM and the HIGH scenario are about 26 million tonnes and about 113 million tonnes (Section 4.5.1). If compared to the *total production of all organic chemicals* (70, 150 and 300 million t in the three scenarios) the respective percentages are 7% (LOW), 17% (MEDIUM) and 38% (HIGH; Table 4-8).
  The outcome of the scenario LOW is very modest if one considers that already today approximately 10% of the feedstock use of the chemical sector in Germany is bio-based (this is on the higher side or possibly even the maximum of all European countries). In the scenario MEDIUM a respectable number of around 150 facilities of the size of NatureWorks' lactic acid plant (of 180 kt p.a capacity) would be required (this is currently the worldwide largest bio-based chemical plant). Finally, in the scenario HIGH, even nearly 600 plants of this size would be required.
- In 2050 the total product value savings are -0.13, 6.7 and 74.8 billion € in the three scenarios (Section 4.5.2). White Biotechnology hence offers substantial macroeconomic savings in the scenarios MEDIUM and HIGH, while it entails relatively small additional expenses in the scenario LOW.
- For the year 2050, the annual added value of the bio-based chemicals is estimated at about 1.8, 8.8 and 33.2 billion € in the scenario LOW, MEDIUM AND HIGH respectively (Section 4.6.2). In 2010, this added value is between 0 to 2.5 billion €. For comparison, Mc Kinsey estimates an added value of about 11 to 22 billion € for the total of White and Red Biotechnology. In contrast to our calculations the value estimated by Mc Kinsey includes fine chemicals and pharmaceuticals and also enzymatically produced chemicals, which have a large potential compared to fermentation based bulk chemicals especially on the short term (EuropaBio 2003).

Based on the findings presented above we now can draw conclusions. We do so first for environmental impacts and second for economics. Our **conclusions concerning environmental impacts** are:

- In spite of its infancy, White Biotechnology offers clear savings of (non-renewable) energy use and GHG emissions already TODAY and substantial further improvements are, in principle, possible for the FUTURE. To realize these improvements, measures need

to be taken with regard to firstly the feedstock choice, secondly the biotechnological step (fermentation) and thirdly product separation and purification.

- With regard to feedstocks the following conclusions have been drawn:
  - Fermentable sugar from sugar cane would be the preferred feedstock because it requires the lowest amount of NREU and leads to the lowest release of GHG emissions.
  - Since sugar cane cannot be cultivated in Europe for climatic reasons, a possible option would be to import fermentable sugar from this source as feedstock for chemical processes. This is not in the interest of European farmers which raises the question about its implementability in view of the hitherto great importance of agricultural policy and its subsidy system in the European Union.
  - As an alternative, European chemical companies could build their production plants in tropical countries with ample sugar cane production. This, however, raises questions about the limits of such a strategy in view of the availability of land in the longer term (including its demand for food and feed), about the impacts on natural biodiversity (not analyzed in this study) and also about social sustainability in view of the low wages paid to workers on sugar cane plantations and the dismal working conditions.
  - Fermentable sugar from lignocellulosics could become a serious option for Europe provided that successful R&D is set up and executed. Under these conditions, lignocellulosics could become a source of cheap and ample amounts of fermentable sugar in Europe, with clear environmental advantages compared to fermentable sugars derived from starch (lower NREU, lower GHG emissions and clearly lower land requiements due to the use of waste streams).
  - For the time being, fermentable sugar (dextrose) from starch is the cheapest indigineous raw material for White Biotechnology processes in Europe and it is available in large quantities. In Europe, fermentable sugar can also be produced from sugar beet but at higher production cost. Apart from its lower cost, starch has key advantages that apply to a large extent also to other renewable raw materials, i.e. it contributes to a substitution to fossil fuels, it is climate neutral (except for the climate effects of the fuels of tractors and transportation and related to fertilizer production and use), is safe to transport and to use and is has a stable price compared to oil.
- With regard to the contribution to possible climate protection goals for the longer term, the conditions in the scenario LOW do not allow White Biotechnology to offer any meaningful contribution. In contrast, the potential contribution is substantial in the scenarios MEDIUM (0.19-0.30% p.a. NREU savings) and in particular, in the scenario HIGH (0.40-0.77% p.a. NREU savings).[117] While these results show that the saving opportunities are substantial at the level of the chemical industry, new technology in the chemical sector *alone* cannot be expected to reduce, in a major way, nation-wide (or EU-wide) environmental impacts. The impacts of White Biotechnology for reducing environmental impacts could become clearly larger than indicated by this report if White Biotechnology is applied to fuel production (e.g., ethanol) which is beyond the scope of this study (exception: energy savings per unit of agricultural land used, see above).
- There are several environmental and health effects that have not been studied in this report (and partly cannot be studied without fundamental research) but that are likely to be important to take into account. Among them are allergic effects to humans, biodiversity

[117] Exemplary calculation, for upper value in scenario HIGH (31% savings in 2050 compared to reference): $1 - (100\% - 32\%)^{1/50} = 0.77\%$ p.a.

loss in the natural environment (e.g., in the case of large-scale biomass production in Latin America) and the availability of process water; in addition, especially the risks from genetic engineering should be considered which will be discussed in Section 7.3.

With regard to **economics**, a number of **conclusions** can be drawn from the product-by-product analysis and the scenario analysis.

- Firstly, it is important to realize that the differences in feedstock costs across the globe are very substantial (around a factor of 5), that these differences have a strong impact on the production costs of chemicals, and that fermentable sugar from sugar cane would be the preferred feedstock from an economic perspective. Policy makers need to take into account that Europe is in a disadvantageous situation with regard to feedstock costs.
- As a consequence, the large-scale production of White Biotechnology products will most likely occur first in countries with low prices of fermentable sugar (in particular, in Latin America). The development of a White Biotechnology industry in these countries represents an opportunity for European industry and European R&D. For economic reasons, it is more advantageous to set up production facilities in countries with low-cost fermentative sugar compared to the production in Europe using imported, low-cost fermentable sugar or crops. The products produced in countries with cheap fermentable sugar will be traded world-wide and will be imported to Europe. In spite of the variety of currently available feedstocks and unexploited potentials in Europe, a boost for White Biotechnology in Europe is only expected if the conversion of lignocellulosics to fermentable sugars becomes a new, widely available low-cost source for fermentable sugar in Europe. To summarize, European industry is likely to develop White Biotechnology in Europe, to apply it first on a large scale abroad and finally to exploit its opportunities in Europe.
- If actively promoted, White Biotechnology can contribute substantially to lower production cost and hence to the wide-scale introduction of bio-based products. If implemented successfully, White Biotechnology offers substantial macroeconomic savings of up to around 75 billion € (scenario HIGH) in Europe because the same demand can be satisfied at lower cost. These macroeconomic savings contribute to improved international competitiveness of the European chemical sector and more generally, of European industry, thus helping to defend employment possibilities in Europe.

We will revert to some of these conclusions when drawing overall conclusions and deriving recommendations in Section 7.5.

7.1.3 Risks of biotechnology for the production of bulk chemicals

When discussing the risks related to the application of biotechnology for the production of organic bulk chemicals a distinction must be made between firstly conventional risks and secondly risks related to Genetically Modified Organisms (GMO).

Conventional risks

In Section 5.1 we developed and applied a generic approach for the assessment of conventional risks related to the production of petrochemicals and White Biotechnology chemicals. With *conventional risks* we refer to risks to human health and life, thereby taking into account accidents, illnesses and external risks imposed on the public due to emissions and technological disasters. Five cases are studied, i.e. polytrimethylene terephthalate (PTT), polyhydroxyalkanoates (PHA), polyethylene terephthalate (PET), polyethylene (PE) and ethanol. The approach combines rather classical risk assessment methods (largely based on chemistry) as developed by the Life Cycle Assessment (LCA) community with statistical information on technological disasters, accidents and statistics on work-related illnesses. The method covers the *total process chain* for petrochemical and bio-based products *from cradle to grave*. It comprises the sectors agriculture, extraction and refining of fossil fuels, chemical industry, power generation, transport and waste management.

It has been found that by far the most important source of risks (expressed in terms of Years of Lost Life, YOLL) are external risks caused by regular release of emissions to the atmosphere, followed by pulmonary health problems of workforce and accidents of the workforce (fatal accidents and accidents with more than three days of absence). External risks imposed on the public due to technological disasters are found to be negligible.

According our calculations the conventional risks related to all White Biotechnology products studied are lower than for the petrochemical products. While these average results are in favour of bio-based production the uncertainties involved in the assessment are large to very large. Taking into account the uncertainties with respect to the ranges of input data, the (incomplete) coverage of the emissions by EPS 2000 and the uncertainties of the assumptions made in this study, the differences in the results between bio-based and petrochemical products (although in favor of bio-based production) definitely fall into the uncertainty range. Therefore, in view of the considerable uncertainties involved, application of our method leads to the conclusion that the conventional risks of biotechnologically produced chemicals (risks related to genetically modified micro-organisms and crop plants excluded) are comparable to those of chemicals derived from fossil fuels.

This finding is partly determined by the methodology which i) yields results that are largely driven by lower energy use and ii) makes use of generic risk factors for chemical industry. The latter is justified because the type of raw materials and the type of processes do not differ essentially from each other. However, if White Biotechnology materializes, new raw materials, intermediates and final products will be handled. This inevitably leads to new risks which will need to be identified and mastered. As experienced in the petrochemical industry in the past, industrial accidents will also happen in the emerging bio-based sector. There is, however, no reason to assume that the risks in the emerging bio-based sector cannot be mastered. To minimize the frequency and the hazard of incidents suitable safety procedures needs to be developed for the White Biotechnology industry.

Risks related to Genetically Modified Organisms

For the industrial production of bulk chemicals like polylactic acid and polyhydroxyalkanoates, the use of genetically modified organisms (GMOs) have been proposed. These compounds can be produced by genetically modified (GM) micro-organisms

like bacteria and yeasts or GM plants. The processes (production facilities) differ decisively in these two cases. To assess risks associated with the application of GMOs for each production route, different scenarios must be evaluated. Production of polylactic acid or polyhydroxyalkanoates by enzymes extracted from GMOs or by GM micro-organisms, will take place in closed fermentation systems. In contrast, the production of these compounds in GM plants will take place on open fields. Therefore, possible risks related to the application of GMOs in bulk chemical production will differ depending on the type of modification. In Section 5.2, an overview of potential risks linked with application of GMOs for bulk chemical production was given. The evaluation of possible risks associated with GM plants has been limited to effects during the primary production stage.

Risks generally proposed to be associated with the use of GMOs are: uncontrolled growth, extinction of species, loss of biodiversity, food poisoning and accumulation of inedible compounds in food chains. Risk, calculated from the equation potential hazard times the chance on occurrence, will vary depending on the production route. In closed reactors escape of GM micro-organisms will only occur after accidents. However, wastes from fermentors may be a possible route for release of GM micro-organisms to the environment. For risk evaluation studies, accidental releases and escape via waste products must be emphasized. For production of bulk chemicals by GM plants in open fields, permanent escape of GM materials is realistic.

Proposed order of events after GM-micro-organism release from closed vessels will be: dispersion of the GM strain, survival and persistence in other habitats and recombinant DNA transfer which finally may accumulate in food or environmental impact. Data extracted from scientific publications revealed that *Alcaligenes eutrophus*, *Aeromonas hydrophila* and *Arxula adeninivorans* were genetically modified with polyhydroxyalkanoate production genes in the past. Risk assessment based on these constructs can be performed for different accident or waste management scenarios. The proposed order of possible events after escape of GM plants, or plant products, from open production fields are: spread and out crossing, growth in other agricultural fields or nature which finally may accumulate in food chain contamination or species diversity loss in nature. From data extracted from scientific literature it appeared that flax and tobacco were modified with polyhydroxyalkanoate production genes in the past. Risk assessment studies based on these constructs must be performed in combination with the production environment where these plants are intended to be grown.

Risk assessment studies must be based on combined evaluations of recombinant construct and production environment. Because production environments are not yet defined, it was not possible to present an accurate risk assessment on these examples. However, in general it can be concluded that proposed applications of enzymes from GMO's and GM micro-organisms in closed systems will entail the lowest risk. Safe containment and inactivation of genes is very important because not all possible implications caused by the release of genes can be foreseen as a result of the complexity of the mechanisms and interrelations involved. Particular attention will have to be paid to potential risks related to the management of large volumes of reactor wastes containing living GM micro-organisms. Adequate risk considerations will have to be applied here. Further, knowledge on microbial communities in different ecological habitats (ecological baseline) was identified as an important knowledge gap which may restrict clear statements on actual risks.

In conclusion, the risks related to the use of genetically modified organisms in White Biotechnology are manageable if adequate precautionary measures are taken. In view of

existing knowledge gaps, the specification of these measures requires further work. The challenges are larger for Green Biotechnology compared to White Biotechnology, which is hence closer to large-scale production in chemical industry.

7.1.4 Public and stakeholder perception of White Biotechnology

It is well known from earlier cases (e.g., nuclear energy and GMOs) that public acceptance can be decisive for the market development of a new technology or product (Section 6.1). In the past, the European public revealed to be very sensitive to biotechnological innovations and it is therefore reasonable to study the possible public response to the production of bulk chemicals from renewable resources by means of White Biotechnology.

In a first step, a comprehensive search and review of existing studies on the public perception of biotechnology and related issues was carried out (Section 6.2 and 6.3). Most of the existing reports on public perception of biotechnology concern *Green Biotechnology* (the application of genetic modification to crop plants and micro-organisms in agriculture) and *Red Biotechnology* (the application of genetic modification to humans in medicine). Five studies were found which allow to draw some conclusions related to White Biotechnology chemicals, even though the subject matter was fully not congruent with that of the BREW study (the conclusions will be discussed below). Due to the very limited number of studies providing insight into the public perception of White Biotechnology, a second step was taken: CERISS and Fraunhofer ISI carried out a survey on opinions and attitudes expressed by selected stakeholders through a questionnaire (Section 6.4). The stakeholders included in the survey were corporate officials, academics, researchers, government officials and non-governmental organisations (NGOs). The survey was conducted among these stakeholders instead of a sample of the public because the debate about White Biotechnology is, at present, still largely confined to these circles and because the knowledge in the public about the options and implications of White Biotechnology was considered to be too low to arrive at meaningful results. In addition, the stakeholders are in the position to strongly influence strategic decisions and public perception of these issues, and therefore may be considered as a suitable proxy for prevailing short to medium term attitudes and perceptions of industrial biotechnology. The BREW survey covered the production of bio-based chemicals by means of White Biotechnology and also Green Biotechnology was included for reasons of comparison. The results allowed to derive a qualitative ranking of the key determinants of public and stakeholder perception.

Using the results of the BREW survey and of the studies (especially BMBF project by Voß et al. 2002 and the Kassel Pilot Project by Lichtl 2003 but also the Eurobarometer surveys on biotechnology by Gaskell et al. 2002 and NatureWorks' Graptine study, 2003) we draw the following conclusions:

- Comparing the level of sustainability across technologies, White Biotechnology chemicals reach **practically the same scores as renewable energy**, among them bioenergy (this conclusion is supported by the BREW survey and the Kassel survey). This finding is very important in view of the generally very positive public perception of renewable energy.
- The main reason for this clearly positive overall view of bio-based chemicals is the understanding of **substantial environmental benefits** (this conclusion is supported by the BREW survey and the Kassel survey; for Green Biotechnology it is also supported by the

BMBF study; and for enzymes produced by genetically modified enzymes by Eurobarometer). The expectation of substantial environmental benefits is dominated by the positive connotation made between bio-based chemicals and the reduction in fossil energy use and greenhouse gas emissions. In contrast, most other factors, among them economic considerations, geopolitical factors (supply security) and risks to environment (biodiversity) and to health do not seem to be of major importance for public perception.

- It therefore seems safe to say that the **overall level of acceptance for the biotechnological production of industrial products is rather high.** At the same time important differences exist among the biotechnological production options with
  - White Biotechnology (regardless whether *with* or *without* genetic engineering) being clearly favoured over Green Biotechnology
  - non-industry respondents favouring non-gene modified microorganisms over gene modified microorganisms.

  These differences should be taken seriously.
- Comparisons across different types of packaging materials as surveyed in the Kassel project indicate that the production of chemicals from biofeedstocks instead of fossil fuels **contributes clearly positively to the chemical industry's image in the public.**
- As an overall summary, a **basically positive attitude** toward the development of White Biotechnology for bulk chemicals can be expected due to the prospects of large environmental benefits as a consequence of the use of renewable raw materials. This conclusion is, however, based firstly on studies which partly have a different scope than the BREW study and secondly on the BREW survey among stakeholders which may differ from the perception of the public. More certainty can only be ensured by means of a study dedicated to public perception.
- A further important implication of the positive attitude towards White Biotechnology being based on the promise of clearly lower environmental impacts is that this technology **must live up to this expectation** (with all its facets, i.e. including not only energy use and greenhouse gas emissions but also all other major environmental impacts such as risks related to genetically modified organisms). **Transparency** about the status and prospects in these matters is very likely to be critical for a continued positive perception.

7.2 Conclusions

In this study we investigated the opportunities and risks of the biotechnological production of bulk chemicals from renewable resources in Europe. As a basis for drawing conclusions we summarize the findings as follows:

- White Biotechnology for bulk chemicals production is **primarily an economic challenge** while it **offers very substantial opportunities for the chemical industry to reduce their non-renewable energy use, greenhouse gas emissions** and related environmental impacts. Nearly all of the products studied are environmentally attractive (non-renewable energy use and greenhouse gas emissions) already with current technology. This concerns the comparison of White Biotechnology chemicals with conventional organic chemicals derived from oil and natural gas. Moreover, White Biotechnology chemicals score clearly better than liquid biofuels (ethanol) with regard to land use efficiency (non-renewable energy savings per unit of agricultural land used). The *economic* challenge of White Biotechnology chemicals in competition with their petrochemical counterparts is closely

linked to technological progress. In conclusion, technological breakthroughs (both in the bioprocess step and in product separation and purification) are more important in order to achieve economic attractiveness than to improve environmental attractiveness.

- **Conventional risks** of biotechnologically produced chemicals (risks related to genetically modified micro-organisms and crop plants excluded) are comparable to those of chemicals derived from fossil fuels); however, if White Biotechnology materializes, new raw materials, intermediates and final products will be handled and as a consequence, suitable safety procedures need to be developed.
- The **risks related to the use of genetically modified organisms** in White Biotechnology are manageable if adequate precautionary measures are taken; in view of existing knowledge gaps, the specification of these measures requires further work; the challenges are larger for Green Biotechnology compared to White Biotechnology, which is hence closer to large-scale production in chemical industry.
- Stakeholders and the public seem to have a **basically positive attitude** towards organic chemicals made from White Biotechnology, with environmental considerations and the use of renewable raw materials primarily determining this perception. This conclusion is, however, based firstly on studies which partly have a different scope than the BREW study and secondly on the BREW survey among stakeholders which may differ from the perception of the public. While more certainty can hence only be ensured by means of a study dedicated to public perception, the available information indicates that public perception is no critical issue and is, on the contrary, supportive under current circumstances.

We conclude from the above that advanced technology (White Biotechnology and downstream processing) is a crucial enabler while there is no serious concern regarding risks and even rather positive feedback regarding public perception. This means that White Biotechnology chemicals represent a prime candidate for ambitious R&D funding at the company and at the state/European level. At the same time, the chances of success must be taken into account. The chances of success are determined by both the progress made in White Biotechnology including downstream processing and the (competing) progress made in the production of fossil-based chemicals:

- Regarding the first aspect (progress made in White Biotechnology plus downstream processing) it should be kept in mind that the **assumptions made in the BREW study** for the future with regard to the bioprocess (see especially Table 3-2) and downstream processing are crucial for the outcome of the calculations. The assumptions are partly judgement-based and they would need to be underpinned by more detailed analyses. If some of the assumptions turn out to be overoptimistic this does not necessarily mean that the conclusions would change because beyond a certain threshold level (e.g., for productivity; see Box 3-3) the consequences for energy use and economics become marginal. Further investigations would be required to arrive at more solid conclusions in such cases.
- Regarding the second aspect (progress made in the production of fossil-based chemicals) it should be kept in mind that **innovations in fossil-based chemicals production** have not been taken into account in the BREW project while they could decisively influence the degree to which White Biotechnology will be implemented in the chemical sector. In oil and natural gas-based chemical industry most changes are gradual, making step changes improbable. The largest menace to (bio-based) White Biotechnology could be the production of olefins from coal if it turns out to be economically superior (first

comparative analyses on these options are in preparation; Ren et al., forthcoming). The most obvious options of coal-based olefin production are the conversion of syngas either to an equivalent of oil-based naphtha for further processing in steam crackers or to methanol for further processing in methanol-to-olefin processes.

We conclude from our analysis that the following **four core requirements** must be fulfilled in order to make clear steps towards a bio-based chemical industry, namely:

1. **Substantial technological breakthroughs must be realized in the bioprocess step.**
2. **Major progress must be made in downstream processing.**
3. **Prices for fossil fuels must be high.**
4. **Prices for fermentable sugar must be low.**

Next, we specify the four core requirements and we provide suggestions for measures which could be taken:

- Regarding the required technological breakthroughs in the bioprocess step, especially clearly higher productivities and concentration must be achieved. To this end, it is recommended to develop **roadmaps with target values for the key parameters** productivity, concentration and yield; such target values could be developed **for 5-year periods in the next 20 years** and could give some **guidance to public R&D programmes**.
- Regarding the required progress in downstream processing, all options should be developed further but membrane technologies should be given most attention. It is proposed to proceed by analogy to the bioprocess field, i.e. to develop **roadmaps with target values for the longer term.** In order to make fast progress in downstream processing and also in bioprocesses (preceding point), best possible use must be made of the extensive knowledge in chemical technology which puts Europe into a rather good position compared to other world regions. In view of increasing competition and with the goal of maximum cost-effectiveness in R&D, co-ordination with research programmes in the U.S. and Japan should be sought for (also with China, Latin America and India as soon as intellectual propertyP issues allow), possibly leading to an international division of tasks.
- The requirement of high prices for fossil fuels is possibly the most difficult to realize in practice. While high fossil fuel prices have been experienced in 2005 (with an average yearly crude oil price of nearly 50 US$/barrel),[118] further increases would be necessary in order to clearly increase the market share of bio-based chemicals. However, it does not seem realistic to envision a European policy actively aiming for high oil and gas prices since this could be detrimental for the competitiveness of European chemical industry as a whole and for other economic sectors. On the other hand, smaller steps, e.g. implemented in the context of the Emission Trading scheme, could possibly create desired incentives for the gradual structural change towards bio-based chemicals.
- With regard to the required low prices for fermentable sugar it is important to realize that Europe is at a relative disadvantage compared to its competitors because the cheap production of fermentable sugar from sugar cane is not possible for climate reasons and

[118] The average "Free On Board" price of crude oil imports to the USA amounted to 47.5 US$/barrel (http://www.eia.doe.gov/pub/oil_gas/petroleum/data_publications/petroleum_marketing_monthly/current/txt/tables01.txt)

fermentable sugar from starch is relatively expensive. Several strategies are thinkable under these conditions: Europe may, for example, decide to

- find a suitable financial supoport scheme to lower the cost of fermentable sugar from starch (one option may be a reduced VAT rate) and/or
- allow free trade of fermentable sugar used for White Biotechnology processes and/or
- support R&D for the production of fermentable sugars from lignocellulosic feedstocks.

The latter is in any case recommended because our results indicate that lignocellulosic feedstocks could be a major enabler for White Biotechnology in Europe for both environmental and economic reasons.

Next to the four core requirements discussed above the **following important accompanying activities** must be tackled if the decision is made to actively support White Biotechnology chemicals:

- A White Biotechnology community should be established in order to realize efficient co-operation among the various stakeholders in all stages of value chain.
- A culture of open dialogue should be created among the stakeholders, enabling transparency about the interests, drivers and possible obstacles and conflicts
- Accompanying strategic studies and evaluations should be conducted, including also in-depth techno-economic and environmental analyses, risk assessment and continuous monitoring of the public perception (e.g., Eurobarometer) and the results should be used for readjustment of the strategy.

To conclude, we strongly recommend to **develop an integrated White Biotechnology strategy** taking into account the four core requirements and the proposed accompanying activities, provided that the European Union arrives at the conclusion to actively support White Biotechnology.

8. References

Note: The references are given by chapter.

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9. Abbreviations

a	year
CH_4	methane
CO_2	carbon dioxide
CHP	combined heat and power (plant)
d	day
ECCP	European Climate Change Programme
EPS	expanded polystyrene
eq.	equivalents
g	grams
GHG	greenhouse gas emissions
GJ	Gigajoule (10^9 joules)
GM	Genetic modification, genetically modified
ha	hectare
HDPE	High density polyethylene
HHV	Higher heating value
kg	kilogramme
kt	kilotonne
l	liter
LCA	life cycle assessment
LHV	Lower heating value
LDPE	low density polyethylene
LLDPE	linear low density polyethylene
MD	Machine Direction (test method for elongation, tensile strength)
MJ	Megajoules (10^6 joules)
Mt	Megatonne (10^6 tonnes)
m^3	cubic metre
MSWI	municipal solid waste incineration plant
N_2O	nitrous oxide
NREU	Non-renewable energy use
NRGHG	Greenhouse gas emissions from non-renewable fuels or feedstocks
P&M	Policies and Measures
PA	polyamide (nylon)
p.a.	per annum
PCL	polycaprolactone
PDO	1,3-propanediol
PE	polyethylene
PET	polyethylene terephthalate
PHA	polyhydroxyalkanoates
PHB	polyhydroxybutyrates
PJ	petajoule (10^{15} joules)
PLA	polylactide, polylactic acid
PO_4	phosphate
PP	polypropylene
PS	polystyrene
PTT	polytrimethylene terephthalate
PUR	polyurethane
PVOH	polyvinyl alcohol

REU	Renewable energy use
RRM	Renewable raw material
R&D	Research and Development
SO_2	sulphur dioxide
t	metric tonnes
TJ	tetajoule (10^{12} joules)
t p.a.	metric tonnes per annum
TPS	thermoplastic starch
, (comma)	thousand separator
. (point)	decimal separator

Conversion factors

1 metric tonne = 2205 pounds
1 metric tonne = 1.102 tons
€ 1 = US $ 1.0 (unless otherwise stated)

Density of air: 1.29 kg/m_N^3

Country Groupings

EU-15	European Union-15: Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Italy, Luxembourg, Netherlands, Portugal, Spain, Sweden, United Kingdom.
EU-25	EU-15 plus 10 accession countries: Cyprus, the Czech Republic, Estonia, Hungary, Latvia, Lithuania, Malta, Poland, the Slovak Republic and Slovenia
W.Europe	EU-15, Faroe Islands, Gibraltar, Iceland, Malta & Gozo, Norway, Switzerland

10. Glossary

Bio-based chemicals	In general, bio-based chemicals are all chemicals that have been produced (fully or partially) from renewable feedstocks. For convenience, we use the term "*bio-based chemicals"* in this study as abbreviation for bio-based *bulk* organic chemicals produced by means of White Biotechnology. We refer to these products also as "White Biotechnology products".
FUTURE	Describing the situation in 2-3 decades from now
Green Biotechnology	Application of biotechnology for the production of genetically modified crops (nowadays mostly for food and feed products)
HIGH	Stands for a scenario with favourable conditions for bio-based chemicals (up to 83 US$/barrel, approx. 70 €/t sugar and 3.0% p.a. physical growth of chemicals)
Industrial Biotechnology	Synonym for White Biotechnology (see below). The term "White Biotechnology" is primarily used in Europe while "Industrial Biotechnology" is the term used in the U.S.
LOW	Stands for a scenario with unfavourable conditions for bio-based chemicals (oil price up to 30 US$/barrel; sugar price of up to 400 €/t; 0% p.a physical growth in the chemical sector)
MEDIUM	Stands for a scenario with medium conditions for bio-based chemicals (up to 66 US$/barrel, up to 200 €/t sugar and 1.5% p.a. physical growth of organic chemicals)
Non-renewable energy use (NREU)	Total of fossil and nuclear fuels but excluding renewable energy (mostly referring to the system "cradle-to-factory gate" in this report because it has been shown in Chapter 3.4.2 that the conclusions by and large coincide for other system boundaries and for the system "cradle-to-grave".
Red Biotechnology	Application of biotechnology for medical purposes
White Biotechnology	Application of fermentation and enzymatic processes for the production of chemicals and fuels; White Biotechnology may or may not make use of genetically modified organisms.
White Biotechnology products	See above definition for"bio-based chemicals"

Appendices

Appendix 1: Calorific values, carbon content and CO_2 emission factors of fuels and feedstocks

Includes petchem feedstocks, intermediates and products, bio-based feedstocks (and intermediates, and products where applicable (in most cases this will be calculated in BREWtool); auxiliaries and catalysts; and fuels.

A1.1 Calorific values of lignocellulosic feedstocks

Product	LHV GJ/t dm	HHV GJ/t dm*)	Carbon content t C/t	
Wood, coniferous tree	19.3	20.8	0.497	LHV from [1]; Carbon content from [2]
Wood, deciduous trees	18.1	19.5	0.475	LHV from [1]; Carbon content from [2]
Corn stover	17.7	19.1	0.457	[2]
Wheat straw	17.2	18.6	0.401	[2]
Hemp	17	18.4	0.461	[2]
Average value for biomass (value chosen in BREW)		**19.0**	**0.45**	

*) Estimate based on LHV from Dubbel (dm=dry matter).

[1] DGfH (Deutsche Gesellschaft fuer Holzforschung)
[2] Fachagentur Nachwachsende Rohstoffe, Leitfaden Bioenergie

A1.2 Calorific values, Carbon content (as equivalent CO_2 emissions), $NREU_{cf}$, GHG_{cg} and Price for BREWtool inputs by category

	Formula	Molar mass	Unit	Calorific value, HHV	Carbon (C) embodied in product as CO_2 equiv.	Total NREU, HHV basis, cradle-to-factory-gate	CO_2 emission from oxidation of product; fossil-based only	GHG emissions cradle-to-factory gate	GHG emissions cradle-to-grave	Sources (for energy, emissions, land)	Price (various sources)
		g/mol		GJ/t	t/t	GJ/unit	t CO_2/unit	t CO_2 eq./unit	t CO_2 eq./unit		EUR/ unit
010-FEEDSTOCKS and INTERMEDIATES, PETCHEM-BASED											
01-1,3-Propanediol	C3H8O2	76.10	t	25.18	1.735						2414
01-1,4-Butanediol	C4H10O2	90.12	t	29.01	1.953						1110
01-Acetaldehyde	C2H4O (l)	44.05	t	27.06	1.998	43.58	1.998	0.940	2.938	C-STREAMS	772
01-Acetic acid	C2H4O2 (l)	60.05	t	15.03	1.465	44.68	1.465	1.850	3.315	C-STREAMS	400
01-Acetic acid EcoInv	C2H4O2 (l)	60.05	t	15.03	1.465		1.465	1.850	3.315	ecoinvent	400
01-Acetone	C3H6O (l)	58.08	t	30.84	2.273	62.96	2.273	1.900	4.173	C-STREAMS	417
01-Acetylene	C2H2(g)	26.04	t	51.61	3.380	86.34	3.380	1.820	5.200	C-STREAMS	1773
01-Acrolein	C3H4O (l)	56.06	t	28.15	2.354						2754
01-Acrylamide, 50% soln, 100% basis	C3H5ON	71.08	t	24.82	1.857						2340
01-Acrylic acid	C3H4O2	72.06	t	18.70	1.832	47.15	1.832	1.670	3.502	C-STREAMS	880
01-Acrylonitrile	C3H3N	53.06	t	33.16	2.488	72.17	2.488	2.120	4.608	C-STREAMS	845
01-Adipic acid	C6O4H10 (s)	146.14	t	19.34	1.806	85.54	1.806	3.960	5.766	C-STREAMS	1090
01-Adiponitrile	C6H8N2	147.14	t	34.27	2.441						875
01-Ammonia from heavy oil	NH3 (g)	17.03	t	22.47	0.000	41.38		2.590	2.590	C-STREAMS	116
01-Ammonia from natural gas	NH3 (g)	17.03	t	22.47	0.000	35.05		1.680	1.680	C-STREAMS	116
01-Benzene	C6H6 (l)	78.11	t	41.83	3.380	67.32	3.380	0.770	4.150	C-STREAMS	401
01-Benzene APME	C6H6 (l)	78.11		41.83	3.380	67.72	3.380	1.527	4.906	APME	401
01-Butadiene	C4H6	54.09	t	46.97	3.254	61.48	3.254	0.710	3.964	C-STREAMS	481
01-Butylene	C4H8(g)	56.11	t	49.74	3.137		3.137				750
01-Butyric acid	C4H8O2 (l)	88.11	t	26.44	1.998		1.998				
01-Caprolactam	C6H11NO	113.16	t	32.00	2.333	117.09	2.333	5.250	7.583	C-STREAMS	1320
01-Catechol	C6H6O2	110.11	t	26.08	2.398		2.398				4674
01-Chlorine	Cl2	70.90	t	0.00	0.000		0.000	0.000	0.000		272
01-Crude oil			t	45.80	3.182	49.46			3.578	Frischknecht et. al	
01-Cumene	C9H12	120.19	t	43.40	3.295		3.295				463
01-Cyclohexane	C6H12	84.16	t	49.50	3.137	78.87	3.137	1.615	4.752	C-STREAMS	443
01-Diethylene glycol	C4H10O3	106.12	t	22.37	1.658		1.658				529
01-Dimethyl terephthalate (DMT)	C10H10O4(s)	194.19	t	23.86	2.266						529
01-EGBE			t	43.14	2.226	73.30	2.226	1.810	4.036	various sources	1914
01-Ethane	C2H6	30.07	t	51.90	2.927		2.927				237
01-Ethanol	C2H5OH (l)	46.07	t	29.73	1.910	63.90	1.910	1.990	3.900	C-STREAMS	442
01-Ethyl Acetate	C4H8O2 (l)	47.50	t	26.44	1.998	59.31	1.998	1.889	3.887	various sources	649
01-Ethylbenzene	C8H10 (l)	106.17	t	43.00	3.315	58.39	3.315	0.810	4.125	C-STREAMS	485
01-Ethylene dichloride (EDC)	C2H4Cl2 (g)	98.95	t	14.10	0.889		0.889				254
01-Ethylene from gas oil	C2H4 (g)	28.05	t	50.31	3.137	68.88	3.137	0.920	4.057	C-STREAMS	724
01-Ethylene from light hydrocarbons	C2H4 (g)	28.05	t	50.31	3.137	66.81	3.137	0.840	3.977	C-STREAMS	724
01-Ethylene from naphtha	C2H4 (g)	28.05	t	50.31	3.137	64.81	3.137	0.710	3.847	C-STREAMS	724
01-Ethylene from naphtha APME 2003	C2H4 (g)	28.05	t	50.31	3.137	65.56	3.137	1.30	4.437	APME	724
01-Ethylene glycol	C2H6O2 (l)	62.07	t	19.11	1.418	48.26	1.418	1.670	3.088	C-STREAMS	626
01-Ethylene oxide	C2H4O (l)	44.05	t	29.65	1.998	61.91	1.998	1.667	3.665	various sources	702
01-Ethylmethylketone	C4H8O	72.11	t	35.51	2.441	92.07	2.441	3.258	5.70	various sources	787
01-Formaldehyde			t							C-STREAMS	375
01-Formic acid	CH2O2 (l)	46.03	t	6.10	0.956		0.956				599
01-Fumaric acid	C4H4O4	116.07	t	11.20	1.516						694
01-Glycerol	C3H8O3	92.09	t	18.30	1.433	18.30	1.433	3.258	4.69	various sources	700
01-Hydrogen cyanide	HCN	27.03	t	23.85	1.628		1.628			various sources	1029
01-Hydrogen from NG	H2 (g)	2.02	t	141.77	0.000	180.00			10.080	various sources	1616
01-Hydrogen from NG NREL	H2 (g)	2.02	t	141.77	0.000	203.38			11.888	NREL	1616
01-Hydroquinone from phenol	C6H6O2	3.02	t	26.08	2.398	26.08	2.398		2.40	various sources	3012
01-Hydroquinone from propylene	C6H6O2	4.02	t	26.08	2.398	56.99	2.398	2.751	5.15	various sources	3012
01-Isobutane	C4H10 (g)	58.12	t	49.35	3.028						254
01-Isobutanol	C4H10O	74.12	t	38.38	2.374						463
01-Isobutyraldehyde	C4H8O	72.11	t	35.51	2.441						1157
01-Isopropanol	C3H8O (l)	60.10	t	35.73	2.196						580
01-Isopropyl ether			t		2.584						1025
01-Kerosene	CH1.8	13.83	t	48.41	3.183	52.28	3.183	0.188	3.370	various sources	136
01-Lactic acid	C3H6O3	90.08	t	15.56	1.465						1389
01-Maleic acid	C4H4O4	116.07	t	11.20	1.516						662
01-Maleic anhydride EcoInv	C4H2O3	98.06	t	12.70	1.795	67.72	1.795	5.030	6.825	ecoinvent: maleic	694
01-Methane	CH4 (g)	16.04	t	55.51	2.743		2.743				
01-Methanol EcoInv	CH3OH (l)	32.04	t	22.68	1.373	38.79	1.373	0.680	2.053	ecoinvent:	182
01-Methanol from heavy oil	CH3OH (l)	32.04	t	22.68	1.373	45.30	1.373	1.440	2.813	C-STREAMS	182
01-Methanol from natural gas	CH3OH (l)	32.04	t	22.68	1.373	40.91	1.373	0.930	2.303	C-STREAMS	182
01-Methanol from soft coal	CH3OH (l)	32.04	t	22.68	1.373	46.12	1.373	1.870	3.243	C-STREAMS	182
01-Methanol via BASF process	CH3OH (l)	32.04	t	22.68	1.373	45.69	1.373	1.170	2.543	C-STREAMS	182
01-Methyl Acetate	C3H6O2	33.04	t	22.03	1.782		1.782				1781
01-Methyl Tertiary Butyl Ether (MTBE)	C5H12O	88.15	t	40.19	2.496	77.39	2.496	1.46	3.956	various sources	519
01-Methylenediphenyldiisocyanate (MDI)	C15H10N2O2	250.26	t	28.93	2.637		2.637				2315
01-Naphtha	*C7H16*	*100.20*	t	47.01	3.074	50.77	3.074	0.179	3.253		245
01-Naphtha EcoInv	*C7H16*	*100.20*	t	47.01	3.074	53.25	3.074	0.417	3.491	ecoinvent	245
01-n-Butane EcoInv	C4H10	58.12	t	52.91	3.028	55.51	3.028	0.573	3.601	ecoinvent	396
01-n-Butanol	C4H9OH	74.12	t	36.09	2.374	69.26	2.374	1.890	4.264	C-STREAMS	500
01-n-Hexane	C6H14	86.18	t	51.88	3.063		3.063				328
01-Octanoic acid	C8H16O2	144.21	t	35.51	2.441		2.441				2866
01-Phenol	C6H6O	94.11	t	33.85	2.805	62.43	2.805	1.284	4.089	C-STREAMS	694
01-Potassium carbonate anh	K2CO3	99.11	t	0.00	0.318	0.00					860
01-Propane	C3H8	44.10	t	50.33	2.993		2.993				
01-Propionalaldehyde	C3H6O (l)	58.08	t	31.37	2.273		2.273				1124
01-Propionic acid	C3H6O2 (l)	74.08	t	20.97	1.782		1.782				1014
01-Propylene from naphtha	C3H6 (g)	42.08	t	48.90	3.137	63.40	3.137	0.710	3.847	C-STREAMS	586
01-Propylene from naphtha APME 2003	C3H6 (g)	42.08	t	48.90	3.137	69.50	3.137	1.40	4.537	APME	586
01-Propylene glycol	C3H8O (l)	76.10	t	25.18	1.735		1.735				741
01-Propylene oxide	C3H6O	58.08	t	32.99	2.273		2.273				1090
01-Purified terephthalic acid (PTA)	C8H6O4	166.13	t	19.49	2.119	55.57	2.119	2.238	4.357	various sources	529
01-p-Xylene	C8H10 (l)	106.17	t	42.89	3.315	58.40	3.315	0.770	4.085	C-STREAMS	560
01-Styrene	C8H8 (l)	104.15	t	42.20	3.380	71.12	3.380	1.570	4.950	C-STREAMS	948
01-Succinic acid	C4H6O4(s)	118.09	t	13.41	1.490						5900
01-t-Butanol	C4H10O (l)	74.12	t	35.67	2.374		2.374				525
01-Toluene	C7H8(l)	92.14	t	43.75	3.343	59.26		0.785	0.785	C-STREAMS	397
01-Toluene diisocyanate (TDI)	C9H6N2O2	174.16	t	24.53	2.274		2.274				1850
01-Triethylene glycol	C6H14O4	150.18	t	23.61	1.758		1.758				661
01-Vinyl chloride (VC)	C2H3Cl	62.50	t	19.91	1.408		1.408				648
01-Xylenes mixed	*C8H10 (l)*	*106.17*	*t*	*42.89*	*3.315*						*398*

A1.2 Calorific values, Carbon content (as equivalent CO_2 emissions), $NREU_{cf}$, REU_{cf}, GHG_{cg}, Land use, and Price for BREWtool inputs by category *CONTINUED.*

	Formula	Molar mass	Unit	Calorific value, HHV	Carbon (C) embodied in product as CO_2 equiv.	Total NREU, HHV basis, cradle-to-factory-gate	CO_2 emission from oxidation of product; fossil-based only	GHG emissions cradle-to-factory gate	GHG emissions cradle-to-grave	Sources (for energy, emissions, land)	Price (various sources)
		g/mol		GJ/t	t/t	GJ/unit	t CO_2/unit	t CO_2 eq./unit	t CO_2 eq./unit		EUR/ unit
020-FEEDSTOCKS and INTERMEDIATES, BIO-BASED											
02-Acetic acid ferment	C2H4O2	60.05	t	15.56	1.465						595
02-Ascorbic acid											4630
02-Biomass generic ds			t	19.00	1.648						
02-Cane molasses			t								220
02-Cellulose	C5H10O5	150.13	t	15.56	1.465						
02-Cheese whey			t								71
02-Citric acid Bio	C6H8O7	192.13	t	10.43	1.374						680
02-Coconut oil crude		199.76	t	40.30	2.683	3.19		0.193	0.193	Hirsinger et al.	500
02-Coconut oil fatty acids		199.76	t	40.30	2.683	4.10		0.248	0.248		
02-Corn EU			t	15.90	1.370	8.05			0.678	ecoinvent	118
02-Corn EU 2			t	15.90	1.370	3.97		0.061	0.061	Simapro_BUWAL	118
02-Corn Germ			t			6.30			0.470	Vink (2004)	343
02-Corn Gluten feed			t			6.30			0.470	Vink (2004)	65
02-Corn Gluten meal			t			6.30			0.470	Vink (2004)	242
02-Corn oil crude			t							Hirsinger et al.: LCI	590
02-Corn steep liquor solids			t			6.00			0.470	Vink (2004)	38
02-Corn stover			t	18.05	1.619	0.78			0.070	various sources	26
02-Corn US			t	16.30	1.424	2.530			0.240	Cargill Dow data:	118
02-Corn US avg			t			2.325			0.266	Vink et al. (2004)	130
02-DDGS		0.00	t	0.00	1.465	4.05					146
02-Dextrose-corn-NW publ	C6H12O6	180.16	t	15.56	1.465	6.200			0.400	Vink (2004)	
02-Dextrose-corn-NW publ-ECON_ALLOC	C6H12O6	180.16	t	15.56	1.465	7.8			0.40	Vink (2004)	
02-Dextrose-corn-NW sensitivity-high	C6H12O6			0.00		10.300			0.63	Vink (2005)	
02-Ethanol from corn	C2H5OH (l)	46.07	t	29.73	1.910	24.220		0.129	0.129	SRI 2000-7	1297
02-Ethyl lactate	C5H10O3(l)	118.13	t	23.67	1.862						2205
02-Glycerol crude 80%	80% C3H8O3	73.68	t	12.45	1.172	10.33			0.720	NREL/SR-580-	200
02-Glycerol crude 80%-Amass	80% C3H8O3	73.68	t	12.45	1.172	29.07			2.030	NREL/SR-580-	200
02-Glycerol refined 99.5%	C3H8O3	92.09	t	15.56	1.465	14.95			1.027	BREWtool	700
02-Glycerol refined 99.5%-Amass	C3H8O3	92.09	t	15.56	1.465	37.10			2.575	BREWtool	700
02-Glycerol refined EUR-Amass	C3H8O3	92.09	t	15.56	1.465	23.69		1.082	1.082		700
02-Glycerol refined EUR-Aprice	C3H8O3	92.09	t	15.56	1.465	8.79		0.420	0.420		700
02-Hemicellulase hydrolysate			t								69
02-Lactide NW	C5H6O4	130.10	t	15.35	1.691	45.95		1.163	1.163	NatureWorks data 5	
02-Lipid	C57H104O6	885.45	t	41.75	2.832						
02-Lysine	C6H14N2O2	146.19	t	28.03	1.806	28.03					1440
02-Methanol from bio-syngas	CH3OH (l)	32.04	t	22.68	1.373						227
02-Miscanthus			t	19.15	1.742	0.97		0.14	0.140	Ph.D. Dornburg	n/a
02-Palm kernel oil crude		216.61	t	40.48	2.697	8.91		1.165	1.165	Hirsinger et al.: LCI	
02-Palm oil crude		270.09	t	41.73	2.779	2.64		0.677	0.677	Hirsinger et al.: LCI	
02-Palm oil methyl esters		*285.45*	*t*	*38.63*	*2.620*						*242*
02-Palm oil refined		*269.45*	*t*	*41.78*	*2.776*	*2.90*		*0.745*	*0.745*		*711*
02-Potato slurry proteins			t								228
02-Potato steam peels dm	*C6H12O5*	*164.16*	t	*18.48*	*1.608*					A&F (2003)	34
02-Propionate	C3H6O2	74.08	t	22.03	1.782						1151
02-Protein	C5H7NO2	113.12	t	23.38	1.945						
02-Protein enriched biomass	C5H7NO2	113.12	t	23.38	1.945						400
02-Rapeseed oil crude			t			5.83		2.025	2.025	PhD Patel	501
02-Short rotation poplar			t	19.85	1.742	2.29		0.237	0.237	Ph.D. Dornburg	85
02-Soybean meal, hydrolysed			t								198
02-Soybean oil			t	39.60							429
02-Starch	C6H12O5	164.16	t	18.48	1.608			1.608	1.608		
02-Starch EcoInv			t	*15.89*	*1.383*	18.76		1.363	1.363	ecoinvent	
02-Stearic acid	C18H36O2	284.48	t	42.53	2.784						518
02-Sucrose-cane	***C12H22O11***	***342.30***	***t***	***16.22***	***1.542***	***-12.80***			***-0.54***		
02-Sucrose-cane allocated_econ_20%	0	342.30	t	16.22	1.542	1.38			0.107		
02-Sucrose-cane high	C12H22O11	342.30	t	16.22	1.542	-10.63			-0.448	Calc in BREWtool	
02-Sucrose-cane low	C12H22O11	342.30	t	16.22	1.542	-14.97			-0.631	Calc in BREWtool	
02-Sugar cane high			t	4.78	0.482	0.19	0.015		0.015	various sources	
02-Sugar cane low			t	4.78	0.482	0.19	0.015		0.015	various sources	
02-Sugar-lig-NREL-2010	***~ C6H12O6***		***t***	***15.56***	***1.465***	***-4.37***			***-0.161***	***BREWtool***	***33***
02-Sugar-lig-NREL-2010-Miscanthus	***~ C6H12O6***		***t***	***15.56***	***1.465***	***-4.03***			***-0.037***	***BREWtool***	
02-Sugar-lig-NREL-2010-Poplar	***~ C6H12O6***		***t***	***15.56***	***1.465***	***-1.67***			***0.137***	***BREWtool***	***140***
02-Sugar-lig-NREL-2010-Wheat_whole	~ *C6H12O6*			15.56	1.465	-2.82			0.235	*BREWtool*	163
02-Sunflower oil			t								540
02-Tallow		255.10	t	41.88	2.784	24.75		12.978	12.978	Hirsinger et al.: LCI	430
02-Verge grass dm			t	18.08	1.634					composition from	
02-Water	H2O	18.02	t	2.99	0.000						
02-Wheat-whole-plant			t	18.95	1.742	1.65		0.29	0.292	Ph.D. Dornburg	98

A1.2 Calorific values, Carbon content (as equivalent CO_2 emissions), $NREU_{cf}$, REU_{cf}, GHG_{cg}, Land use, and Price for BREWtool inputs by category *CONTINUED.*

	Formula	Molar mass	Unit	Calorific value, HHV	Carbon (C) embodied in product as CO_2 equiv.	Total NREU, HHV basis, cradle-to-factory-gate	CO_2 emission from oxidation of product; fossil-based only	GHG emissions cradle-to-factory gate	GHG emissions cradle-to-grave	Sources (for energy, emissions, land)	Price (various sources)
		g/mol		GJ/t	t/t	GJ/unit	t CO_2/unit	t CO_2 eq./unit	t CO_2 eq./unit		EUR/ unit
030-AUXILIARIES											
03-Acid/base			t			3.22			0.42	Assume 50%	47
03-Activated carbon			t				3.760		3.760		2196
03-Alamine 336	C24H51N	353.67	t	48.68	2.986						4255
03-Ammonia 25%	NH3	17.03	t	27.64	0.000	8.78			0.42		58
03-Ammonium hydroxide	NH4OH	35.05	t	14.97	0.000	14.97					132
03-Ammonium nitrate	NH4NO3	80.04	t	-0.44	0.000	63.22		5.50	5.50		139
03-Ammonium sulphate	(NH4)2SO4	164.19	t	5.72	0.000	54.77		2.53	2.53		50
03-Antifoam SE2		0.00	t	0.00							1146
03-Calcium carbonate	CaCO3	100.09	t	0.00	0.440	1.06		0.070	0.070		284
03-Carbon			t								91
03-Carbon Dioxide EcoInv	CO2	44.01	t	0.00	1.000	8.31	1.000	0.650	1.650	ecoinvent: carbon	57
03-Carbon Monoxide EcoInv	CO	28.01	t	10.11	1.571	59.90	1.571	1.400	2.971	ecoinvent: carbon	175
03-Chlorine	Cl2	70.91	t	0.00	0.000				0.000		272
03-Cobalt naphthenate			t								11195
03-Cobaltous sulphate			t								7874
03-Diammonium phosphate	(NH4)2HPO4	132.06	t	0.00	0.000	13.26		0.67	0.670		154
03-Dipotassium phosphate			t								2403
03-EDTA	C10H16O8N2		t								2315
03-Hydrochloric Acid 30% EcoInv	HCl	36.46	t	1.38	0.000	16.09			0.759		84
03-Hydrogen Peroxide 70%	H2O2		t			24.15		1.090	1.090		891
03-Kaolin			t					0.066	0.066		
03-KH2PO4	KH2PO4	136.09	t	0.00	0.000	21.71	0.00	1.34	1.34		900
03-Lime Ca(OH)2 NW	Ca(OH)2	0.00	t	0.00		5.27			0.868	Vink	61
03-Lime Ca(OH)2 EcoInv	Ca(OH)2	74.09	t	0.00	0.000	4.50			0.722	ecoinvent	61
03-Lysine Resin IonX			l								4
03-Magnesium Sulphate EcoInv	MgSO4	120.37	t	0.00	0.000	5.86			0.270	ecoinvent	386
03-Membrane use (high quality)			EUR								100
03-Minerals-H2-ATO		0.00	t	0.00							
03-Nitric acid (diluted)	HNO3	63.01	t	0.00	0.000	14.49		1.20	1.200		88
03-Nitric acid 60%	HNO3	63.01	t	0.00	0.000	0.00					176
03-Nitrogen	N2 (g)	28.01	1000Nm3	0.00	0.000	1.9800				Ikarus (1994)	20
03-Nitrogen EcoInv	N2 (g)	28.01	1000Nm3	0.00	0.000	10.8375		0.491	0.491	ecoinvent: nitrogen	20
03-Nonaromatic Paraffin		13.83	t	48.41	3.18	52.28	3.18	0.19	3.37		661
03-Nutrients PHA			t			5.86			0.270	various sources	243
03-Nutrients-ferment-unspec.			t			5.86			0.270	various sources	50
03-Octanol EcoInv	C8H18O (l)	130.23	t	43.28	2.703	67.40	2.703	2.110	4.813	ecoinvent	2251
03-Oleum 7%			t								132
03-Oxygen	O2 (g)	32.00	t	0.00	0.000	2.7000			0.200	Joosten (2001)	50
03-Perchloric Acid	HClO4	100.46	t	0.00		0.00	0.000		0.000		15120
03-Phosphoric Acid	H3PO4	98.00	t	-5.06	0.000	16.65	0.000	1.340	1.34		278
03-Phosphorus pentoxide	P2O5	141.94	t	-8.12	0.000	-8.12	0.000		-0.601		1307
03-Resin unspecified			t								
03-Sodium Bicarbonate	Na2HCO3	84.01	t	0.00	0.524	0.00	0.000		0.000		370
03-Sodium Bisulfate	NaHSO4	120.06	t	0.00	0.000	0.00					534
03-Sodium Carbonate	Na2CO3	83.00	t	0.00	0.530	15.18		1.29	1.290		139
03-Sodium Chloride	NaCl	58.44	t	-7.04	0.000				0.000		119
03-Sodium Dodecylsulfate	C12H25OSO3Na	288.38	t	27.43	1.831	27.43			0.000		1500
03-Sodium Hydroxide 50% EcoInv	NaOH	40.00	t	-7.07	0.000	20.97			0.981	ecoinvent	89
03-Sodium Hypochlorite 14%	NaOCl	74.44	t	-3.10	0.000	21.90	0.000	1.189	1.189	various sources	125
03-Solvent PHA			t								
03-Solvent-Butyl acetate	C6H12O2	116.16	t	32.07	2.273	32.07					772
03-Solvent-Diisopropyl ether		0.00	t	0.00	#DIV/0!	0.00					1200
03-Solvent-TOPO15/Kerosene85	(CH3(CH2)7)3PO	386.64	t	43.82	2.731	43.82	2.703	2.110	4.813	ecoinvent: solvents,	3000
03-Sulfur dioxide	SO2	64.06	t	0.00	0.000						
03-Sulfuric Acid NW	H2SO4		t			1.47			0.098		32
03-Sulfuric Acid EcoInv	H2SO4	98.07	t	0.00	0.000	1.93			0.113	ecoinvent: sulphuric	32
03-Titanium dioxide	TiO2 (s)		t								187
03-Urea	CH4N2O (s)		t		0.733						229
03-Waste Nylon			t								1613
040-CATALYSTS											
04-A. succinogenes			kg			0.025		0.00165	0.00165	various sources	
04-Alpha amylase			kg			0.025		0.00165	0.00165	various sources	150
04-Cellulase			t			21.71			1.006	Sheehan et al.	1466
04-Enzymes PHA			kg			0.75		0.060	0.060		10
04-Enzymes PHA future			kg			0.125		0.010	0.010		10
04-Gluco amylase			kg			0.025		0.00165	0.00165		20
04-Lipase Candida Rujosa			kg								300
04-Lysine oxidase future			kg			0.125		0.010	0.010		10
04-Lysine oxidase today			kg			0.75		0.060	0.060		100
04-Nickel Catalyst (65% Ni)			kg			0.16		0.02	0.024		30
04-Platinum Catalyst			kg			333300.00		15,300.00	15300.000		
04-Rhodium			g								68
04-Vanadium phosphorous oxide			kg			0.16		0.02	0.02		30
04-Yeast			kg								
050-UTILITIES and FUELS											
05-Biodiesel			GJ	45.40		0.70			0.049	NREL/SR-580-	14
05-Biodiesel-Amass			GJ	45.40		0.64			0.045	NREL/SR-580-	14
05-Biogas			GJ	20.00	2.05						
05-Compressed air			1000mN3			1.00			0.05		6
05-Cooling water			t								0.05
05-Diesel			GJ	45.40		1.08	0.074	0.004	0.078		6
05-Electricity			GJe			2.52			0.117	Eurostat (2003) &	15
05-Fossil fuel by-prod 1			GJ			1.08	0.074	0.004	0.078		
05-Fossil gas 1			GJ			1.07	0.056	0.004	0.060		
05-Fuel oil			t	45.20		48.82	3.345	0.186	3.531		134
05-Hard coal			GJ			1.06	0.093	0.003	0.096		
05-Heavy Fuel Oil			GJ	43.70		1.08	0.074	0.004	0.078		3
05-Heavy gasoline			t								323
05-Hydrogen-rich gas			t								626
05-Inert gas			Nm3								0
05-Light Fuel Oil			GJ	45.20		1.08	0.074	0.004	0.078		3
05-Methane-rich gas											3
05-Natural gas			GJ	49.56	2.743	1.07	0.056	0.004	0.060		4
05-Process water			t								0.25
05-Refrigeration, 0°C			GJrefrig.			0.620			0.027		7
05-Refrigeration, -40°C			GJrefrig.			2.635			0.116		14
05-Residual oil			t								114
05-Soft coal			GJ		1.758	1.06	0.093	0.003	0.096		
05-Steam HP			t			2.73			0.169		12
05-Steam LP			t			2.73			0.169		12
05-Steam MP			t			2.73			0.169		12
05-Syngas H2:CO 1.1:1		14.39	t	16.45	1.356	46.86			2.62		0
05-Syngas H2:CO 1:1		15.01	t	15.61		46.86			2.62		0
05-Syngas H2:CO 2:1		10.67	t	23.57	1.219	46.86			2.62	energy: Chauvel	381

A1.2 Calorific values, Carbon content (as equivalent CO_2 emissions), $NREU_{cf}$, REU_{cf}, GHG_{cg}, Land use, and Price for BREWtool inputs by category *CONTINUED.*

	Formula	Molar mass	Unit	Calorific value, HHV	Carbon (C) embodied in product as CO_2 equiv.	Total NREU, HHV basis, cradle-to-factory-gate	CO_2 emission from oxidation of product; fossil-based only	GHG emissions cradle-to-factory gate	GHG emissions cradle-to-grave	Sources (for energy, emissions, land)	Price (various sources)
		g/mol		GJ/t	t/t	GJ/unit	t CO_2/unit	t CO_2 eq./unit	t CO_2 eq./unit		EUR/ unit
060-WASTE MANAGEMENT/ENERGY RECOVERY									0.000		
06-Biogas export			GJ	20.00	2.05	-1.07			-0.06		
06-Biomass to digestion			t dm	19.00	1.465	-4.94			-0.244	De Mes et al.	
06-Biomass to incineration			t dm	19.00	1.465	-15.60			-0.780	NREL	
06-Calcium sulphate	CaSO4		t								
06-CH4 emission	CH4 (g)	16.04	t	55.51	2.743	55.51	23.000		23.000		
06-CO emission	CO(g)	28.01	t	10.11	1.571	10.11	1.571		1.571		
06-Gypsum	CaSO4*2H2O		t								
06-Gypsum to re-use	CaSO4*2H2O		t			0.034			0.002	various sources	
06-N2O emission	N2O(g)	44.01	t	0.00	0.000		296.000		296.000		
06-OrgIndWaste to digestion			GJ dm	19.00	1.465	-0.28			-0.014	De Mes et al.	
06-OrgIndWaste to incineration			GJ dm	19.00	1.465	-0.46			-0.024	Phylipsen et al.	
06-Sludge to co-combustion			t dm			-4.33			-0.252	Lundin et al. (2004):	
06-Sludge to field			t dm			2.01			-0.032	Lundin et al. (2004):	
06-Solid waste to landfill			t								
06-Starch effluent EcoInv			t effl			0.05			0.014	ecoinvent:	
06-Waste water 1			t COD			7.50			0.555	various sources	930
06-Waste water 2			t effl			0.00			0.00028		0
P1.0-PRODUCTS: POLYMERS											
P1-ABS		1129.49	t	41.92	3.303		3.303				1709
P1-Epoxy resin		284.35	t	33.73	2.785	114.66	2.785	4.680	7.465	C-STREAMS	3086
P1-EPS			t								1391
P1-Lignin (eucalyptus)		212.30	t	24.73	2.193						
P1-Lignin (picea abies)		189.77	t	25.66	2.312						
P1-Melamine resin		198.18	t	18.70	1.332	86.78	1.332	4.130	5.462	C-STREAMS	1323
P1-Nylon-6		113.16	t	32.24	2.333	132.04	2.333	6.130	8.463	C-STREAMS	3228
P1-Nylon-6 APME		113.16	t	32.24	2.333	120.47	2.333	5.500	7.833	APME	3228
P1-Nylon-6,6		226.32	t	32.24	2.333	176.28	2.333	8.570	10.903	C-STREAMS	3402
P1-Nylon-6,6 APME		226.32	t	34.09	2.333	138.62	2.333	6.500	8.833	APME	
P1-P3HA-mcl		170.25	t	36.60	2.584						10000
P1-P3HB		86.09	t	23.76	2.044						10000
P1-P3HV		100.12	t	27.40	2.197						10000
P1-PE LD APME		28.05	t	50.31	3.137	77.80	3.137	1.912	5.048	Boustead (2003)	1000
P1-PET		192.17	t	23.53	2.290	60.24	2.290	2.070	4.360	C-STREAMS	1200
P1-PET Amorph APME		192.17	t	23.53	2.290	80.75	2.290	3.300	5.590	Boustead (2003)	1200
P1-Phenol formaldehyde resin		106.12	t	33.13	2.902	63.97	2.902	1.760	4.662	C-STREAMS	1278
P1-PLA		72.06	t	18.70	1.832	37.06			2.509		2917
P1-PMMA		100.12	t	27.40	2.197		2.197				14814
P1-Polyacrylate		86.09	t	23.76	2.044	84.90	2.044	3.740	5.784	C-STREAMS	1959
P1-Polyacrylonitrile		53.06	t	32.24	2.488	76.60	2.488	2.590	5.078	C-STREAMS	
P1-Polybutylene terephthalate		220.22	t	26.08	2.398		2.398				1636
P1-Polycarbonate		254.28	t	32.11	2.768	86.30	2.768	3.110	5.878	C-STREAMS	3700
P1-Polyetherpolyol			t								3373
P1-Polyethylene		28.05	t	50.31	3.137	74.05	3.137	1.240	4.377	C-STREAMS	1000
P1-Polyethylene HDPE APME		28.05	t	50.31	3.137	76.56	3.137	1.600	4.737	APME	1000
P1-Polypropylene APME		42.08	t	48.90	3.137	72.69	3.137	1.700	4.837	APME	787
P1-Polystyrene		104.15	t	42.20	3.380	76.07	3.380	1.870	5.250	C-STREAMS	1070
P1-Polystyrene APME		104.15	t	42.20	3.380	86.73	3.380	2.600	5.980	APME	1070
P1-Polytrimethylene terephthalate		206.20	t	24.47	2.347						1450
P1-Polyurethane			t			53.40		3.050		C-STREAMS	5760
P1-Polyvinyl acetate		86.09	t	23.76	2.044	59.14	2.044	2.060	4.104	C-STREAMS	1210
P1-Polyvinyl chloride		62.50	t	19.91	1.408	56.45	1.408	2.080	3.488	C-STREAMS	882
P1-PUR flexible		8328.89	t	29.42	2.160		2.160				3452
P1-PUR rigid		2371.70	t	29.24	2.440		2.440				7535
P1-Synthetic rubber		485.30	t	44.86	3.273	70.64	3.273	1.380	4.653	C-STREAMS	1521
P1-Unsaturated polyester/alkyd resin		280.28	t	23.83	2.198	65.07	2.198	2.390	4.588	C-STREAMS	1102
P1-Urea resin		109.60	t	14.69	1.064	50.26	1.064	2.260	3.324	C-STREAMS	1187

A1.3 Energy use for enzyme production

	NREU MJ_{prim}/kg enzyme	Notes on assumptions/system boundaries	Main data source
Aspartic acid dual	2,300	Per tonne of enzyme beads; estimate excludes energy equivalents of raw material inputs	SRI-PEP 241, 2002
Aspartic acid conventional	17,500	Per tonne of enzyme beads; estimate excludes energy equivalents of raw material inputs	SRI-PEP 241, 2002
alpha-Amylase	320	Estimate excludes energy equivalents of raw material inputs AND refrigeration	SRI-PEP 99-6, 2002
Enzyme for ascorbic acid	3,500	Estimate is based on assumption that 0.001 kg enzymes are needed per kg of ascorbic acid; estimate excludes energy equivalents of raw material inputs.	SRI-PEP 99-10, 2002
Enzymes - Generic estimate for present day	2,000	Estimate based on company data on the company's total energy requirements (excluding some raw materials, esp. agricultural produce; but including apart from enzyme production for sale all other company activities, among them extensive R&D)	Personal communication

Table A1.3: Estimates of non-renewable energy use (NREU) for the production of various types of enzymes
Note: These values are larger than the chosen values according to Table 3-11 (see Chapter 3) .

Appendix 2: Power and heat production

A2-1: Public power generation

Data for public power generation for the European Union was taken from IEA Energy Balances for OECD countries 2000-2001 (IEA 2003). Energy use is calculated by summing primary energy consumption in public (grid) electricity plants for all energy types (separately for non-renewable and renewable energy). This is then divided by the figure for gross power generated in public power plants. Summing the specific NREU and REU gives the total energy use in terms of gross power generation; the reciprocal of this gives the efficiency for (gross) power generation (Column 1 in Table A2.1). Net power generated is calculated by subtracting figures in the IEA balance for o*wn use in electricity, CHP (combined heat and power) and heat plants* and *distribution losse*s from the figure for gross power generated. Dividing the total primary energy consumption by the net power generated leads to a higher total specific energy use and a corresponding lower efficiency (Column 2 in Table A2.1). When the energy requirement for energy (ERE) is taken into account the total specific energy use increases by a factor 1.07 (average ERE factor for mixed fuels) and the efficiency of power generation is reduced to 33.4% (Column 2 in Table A2.1).

The total CO_2 emission is calculated by multiplying the primary energy consumption in public electricity plants by the carbon (as CO_2) emission factor for each energy type (IEA 2002) and summing these. Dividing this by gross and net power generated results in the CO_2 emission factors shown in the table. Multiplying CO_2 emissions for net power generation by the ERE factor 1.07 gives the CO_2 factor when ERE is taken into account.

The figures for net power generation performance including ERE (third column) are the ones used in BREW.

Table A2.1 Electricity production and consumption in the EU Chemical Industry

Indicator	Unit	Gross power generation performance	Net power generation performance*)	Net power generation performance and accounting for ERE**)
Non-renewable energy use (NREU)	MJ/MJ_{el}	2.32	2.61	2.79
Renewable energy use (REU)	MJ/MJ_{el}	0.17	0.19	0.20
Total energy use	MJ/MJ_{el}	2.48	2.80	2.99
Efficiency	%	40.3%	35.7%	33.4%
CO_2 emission factor	kg CO_2/GJ_{el}	96	108	116

*) Calculated from Gross power generation performance by deducting own electricity use and power distribution losses

**) Calculated from Net power generation performance by adding energy requirements for energy (ERE; for exploitation, pretreatment and transportation)

A2-2: Cogeneration in the chemical sector

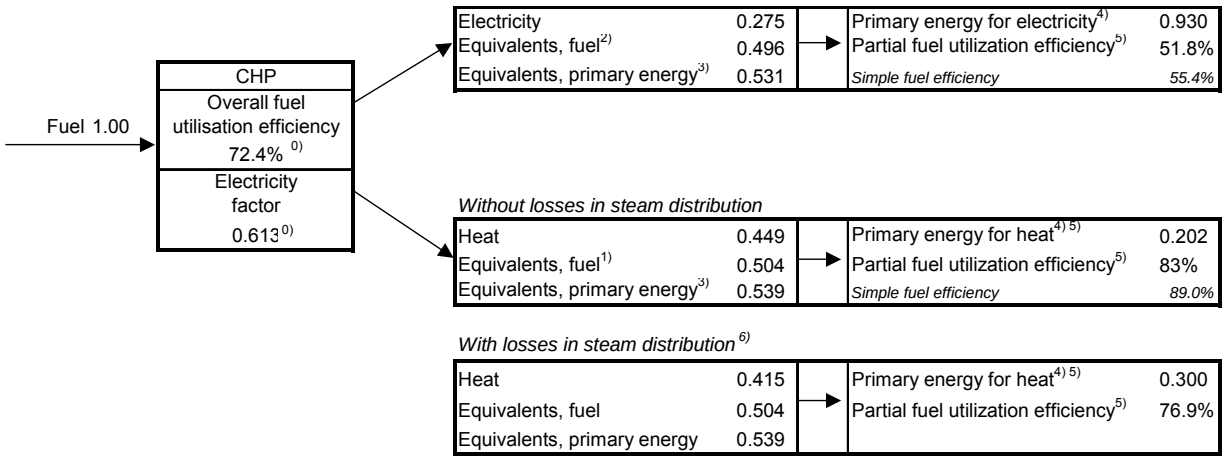
Data for cogeneration of electricity and steam is based on data in the Eurostat publication Combined Heat and Power (CHP) Plant Statistics in the EU, 2000 (Eurostat 2003) together with supplementary figures obtained from an EU representative responsible for the Eurostat publication (Loesenen 2004). The data is presented below as three tables. In Table A2.2, the efficiency of electricity and heat production in the EU Chemical Industry is calculated using data from Eurostat (2003). These are summed to give the overall efficiency. The ratio of electricity to heat produced, also known as the 'electricity factor', is calculated for an average CHP plant.

Table A2.2 Electricity production and consumption in the EU Chemical Industry

	Production		Fuel Input	Overall Efficiency	Electricity/ Heat
	Electricity TJ	Heat TJ	TJ(LHV)		
Own production (CHP)	214800	350500	781300	72%	0.613

Source: Eurostat (2003) with supplementary figures from Loesenen (2004)

The split of final energy in CHP plants between heat and power may then be calculated (Figure A2.1) using the electricity factor and the overall fuel utilisation efficiency. Assuming a simple production efficiency of steam of 89% and including energy requirements for energy, the fuel equivalents for steam are calculated. The remainder of the 1 GJ of fuel input is then allocated to electricity production (fuel equivalents, electricity) and the partial fuel utilization efficiency for CHP electricity calculated.



0) Values for average CHP in the EU acc. to Eurostat (2003) with supplementary figures from Loesenen (2004)
1) Equivalents fuel, calculated via steam production efficiency of 89%
2) Equivalents, fuel, calculated via Energy Conservation Law
3) Primary energy equivalents have been calculated by adding 7% Energy Requirements for Energy (ERE) to "Equivalents, fuel".
4) "Energy overhead", to be added to final energy, in GJ primary energy per GJ final energy
5) including Energy Requirements for Energy (ERE)
6) Assumed steam losses for average maintenance: 7.5%

Figure A2.1 Steam and electricity generation in CHP plants in the chemical industry in EU-15

The CO_2 emissions for fuels used in the EU Chemical Industry are calculated as shown in Table A2.3. Data is based on the extended energy balances for OECD Countries (IEA 2002d). From this an average emission factor is found to be 62 kg CO_2/GJ fuel. Using this average emission factor for fuels, CHP electricity production with efficiency of 51.8% equates to a CO2 emission factor of 120 kg CO_2/GJ electricity.

Table A2.3 CO_2 emissions for an average fuel mix in the EU Chemical Industry

Fuel	Emission factor [2]	Western Europe		
	kg CO_2 / GJ	PJ [1]	%	kt CO_2
Hard Coal	94.6	31	2%	2899
Lignite/Brown Coal/Sub-bituminous Coal	101.2	3	0%	292
Coke oven coke / Lignite coke	108.2	4	0%	430
BKB / Peat briquettes	94.6	4	0%	345
Gas works gas [3]	**47.7**	1	0%	28
Coke oven gas	47.7	6	0%	293
Industrial waste [3]	**73.3**	9	1%	648
Primary solid biomass	0.0	4	0%	0
Natural gas	56.1	978	73%	54863
Refinery gas	66.7	62	5%	4169
Liquefied Petroleum Gas	63.1	30	2%	1867
Other kerosene	71.9	3	0%	241
Gas / Diesel oil	74.1	19	1%	1371
Heavy fuel oil	77.4	94	7%	7298
Naphtha	73.3	52	4%	3780
Petroleum coke	100.8	4	0%	414
Ohter petroleum products [3]	**100.8**	34	3%	3410
Other fuels [3]	**73.3**	1	0%	55
Total		**1337**	**100%**	**82402**
Average emission factor fuels used		**62 kg CO_2 / GJ**		

[1] Excluding feedstock use

[2] Emission factors from IEA (2002d) unless otherwise stated

[3] Emission factors are own estimates

A2-3: Average conversion factors for electricity in the EU chemical sector

The fuel input for electricity production in CHP plants is subtracted from total fuel inputs for electricity consumed in the EU Chemical Industry to give the total consumption of public grid electricity (Table A2.4). The share in primary energy terms of each of the two sources is then calculated. A weighted average generating efficiency for electricity consumed in the EU chemical industry is then calculated by multiplying the efficiency for public electricity generation (from Table A2.1) and CHP electricity generation (from Figure A2.1) by the respective share of total production for each. Average CO_2 emissions are calculated in a similar way.

It should be noted that the CO_2 emission factor is higher for power production in the chemical industry compared to the grid in spite of a higher power generation efficiency in the chemical sector. The reason for this is that a proportion of public power plants operate on nuclear fuels or renewable energy and these two categories do not contribute to CO_2 emissions.

Table A2.4 Weighted average conversion factors for electricity use in the EU Chemical Industry

Electricity production in industry (CHP) and public grid in the EU Chemical Industry

	Fuel Input TJ	Share of total production	Generating efficiency	Weighted average efficiency	CO_2 emission kg CO_2/GJ	Wt Avg CO2 emission kg CO_2/GJ
Own production (CHP)	214800	33.7%	51.8%		120	
Electricity from Grid[0)]	422400	66.3%	33.4%		116	
Total consumption	637200	100.0%		39.6%		117

[0)] Source: IEA (2003): total final consumption of electricity in Chemical and Petrochem Industries

A2-4: Steam Production

The chemical industry uses medium pressure (MP) steam for the majority of applications. Therefore MP saturated steam is assumed unless otherwise stated in the input data. While provision has been made for separate primary energy conversion data to be entered for low pressure, medium and high pressure steam,[119] at present data for medium pressure steam is used for all three categories. Table A2.5 shows the derivation of primary energy equivalents for medium pressure saturated steam. The partial fuel utilisation efficiency for steam production is taken from Figure A2.1.

Table A2.5 Steam production in the EU Chemical Industry

Energy content of steam MP (GJ steam/t steam)[0)]	2.1
Partial fuel utilization efficiency for steam production (including ERE)	76.9%
Conversion factor steam MP (GJ fuel/t steam)	2.73

[0)] Enthalpy of evaporation of medium pressure saturated steam (7 bar abs, 165 °C); from steam tables

[119] Typical specs for steam from Chemsystems (1998): LP: 4 bar, 175 °C; MP: 10 bar, 280 °C; 40 bar, 400 °C.

Appendix 3: Other utilities

A3-1: NREU cradle-to-factory gate and GHG cradle-to-grave

Utility	Unit	NREU [GJ/ unit]	GHG [t CO_2eq/ unit]	Reference
Compressed air	$1000m_N^3$	1.00	0.046	a)
Refrigeration, temperatures around 0°C	$GJ_{refrig.}$	0.62	0.027	a)
Refrigeration, very low temperatures (-40°C and below)	$GJ_{refrig.}$	2.64	0.116	a)
Cooling water	t	0	0	b)
Process water	t	0	0	b)
Nitrogen	$1000m_N^3$	10.8	0.49	c)

a) pers. comms. with P. Radgen, Fraunhofer Institute ISI, Karlsruhe, Germany, May 2004
b) Assumed to be negligible
c) Econinvent 2003

A3-2: Prices for utilities (data for base case in year 2000)

Utility	Unit	Price (year 2000) €/unit	Reference
Crude oil	barrel	25 *)	a)
Natural gas	GJ	4 **)	b)
Electricity	GJ_e	15.2 ***)	c)
LP steam production in the chemical sector	t	12.0	b)
MP steam production in the chemical sector	t	12.0	b)
HP steam production in the chemical sector	t	12.0	b)
Compressed air	$1000m_N^3$	6.0	b)
Refrigeration, temperatures around 0°C	$GJ_{refrig.}$	7.0	b)
Refrigeration, very low temperatures (-40°C and below)	$GJ_{refrig.}$	14	b)
Cooling water	t	0.05	b)
Process water	t	0.25	b)
Nitrogen	$1000m_N^3$	20	b)

*) Stock market price; equal to 4 €/GJ
**) Price paid by the chemical industry
***) Equal to 5.45 Eurocent/kWh

a) Assumptions: 25 US$/barrel and 1.0 €/US$
b) Confidential Industry Sources
c) Eurostat

Appendix 4: Overview of specific energy use by process unit

The data below do not necessarily coincide with the chosen values in Table 3-4 because a calibration step was performed as intermediate step: chosen values according to the tables below were used to estimate the energy use of complete White Biotechnology processes for which detailed energy data was available for the entire plant and some subsections. After comparison of these data with the own calculations for the entire plant final adaptations were made to the energy use per process unit. The final data chosen can be found in Table 3-4. The references are given in Chapter 8 of the report.

Sterilization

Source	Value (kg steam/kg fermentation medium)	Comments
Kalk and Langlykke (1986)	0.2-0.4	Batch sterilization
Kalk and Langlykke (1986)	-	Continuous sterilization. Can cut usage for batch sterilization by as much as
Gerngross (1999)	0.1	Less than 0.1. Calculated for continuous sterilization of medium to 143ºC for 30s, with recapture of 68% of the energy
Bartholomew and Reisman (1979)	0.2	Case study, continuous sterilization
Bartholomew and Reisman (1979)	0.8	Case study, batch sterilization (small scale)
Petrides et al. (1989)	0.2	Case study, continuous sterilizer

Agitation

Source	Value (kW/m3 of	Comments
Kalk and Langlykke (1986)	1 - 3	
Gerngross (1999)	1	
Akiyama et al. (2003)	1	Simulating large-scale production of PHA
Bartholomew and Reisman (1979)	2	Case study, small seed fermentor
Bartholomew and Reisman (1979)	1	Case study, fermentor
Petrides et al. (1989)	1 - 7	Depending on cell concentration, growth rate, product synthesis rate, and broth viscosity
Petrides et al. (1989)	0.2 - 1	Mild agitation
Petrides et al. (1989)	1.5 - 3.5	Antibiotics production by filamentous microorganisms
Petrides et al. (1989)	3.5 - 5.0	Yeast production
Petrides et al. (1989)	> 7	Xanthan gum production
Seider et al. (1998)	2	Heuristic for agitation of slurry with impeller in baffled tank
Fong (1987)	0.2-0.7	Mechanical, Mild Agitation
Fong (1987)	0.2-2.2	Agitator in stirred tank bioreactors. Antibiotics (aerated). Best yeild >1.1
Fong (1987)	3.7	yeast, agitator in stirred tank bioreactors
Fong (1987)	2.2-6	Biomass production, agitator in stirred tank bioreactors
Reisman (1988)	2 - 4	In very general terms, for production fermentors
SuperPro Designer (2004)	0.1	
Industry source	0.5	Minimum value
Industry source	≥1	In presence of solids (e.g. heterogeneous catalyst)
Industry source	8 - 12	Viscous mixtures

Aeration

Source	Value	Value (v v m)	Comments
Kalk and Langlykke (1986)		0.5 - 2	for air deliverd at 100 psia (about 7 atm.), 1 vvm represents power consumption of about 5 kW/m3. Typical aeration rates in fermentors
Gerngross (1999)	4		
Akiyama et al. (2003)		0.5	compressor pressure of about 2500 kPa (about 25 atm.)
Bartholomew and Reisman (1979)		0.2	Case study of the production of a bacterial insecticide
Petrides et al. (1989)		1	Stirred bioreactors, limited to avoid foaming problems
Petrides et al. (1989)		2	Air-lift reactors
Petrides et al. (1989)	6	1	Case study. 6 kW/m3 is the power consumption of compressors
Queener and Swartz (1979)		0.5 - 1.0	production of penicillin G or V
Fong (1987)		0.5 - 1.0	Typical stirred tank bioreactor
Reisman (1988)		0.5 - 1.0	Production of citric acid at a pressure of 1.5 atm
SuperPro Designer (2004)		*0.5*	

Total power for agitation and aeration

Source	Value	Comments
Gerngross (1999)	5	Aerobic fermentations with very high cell densities
Lynd and Wang (2004)	1.5	Representative best-practice electricity requirement for commodity products
Queener and Swartz (1979)	1 - 4	Penicillin production
Charles (1985)	1 - 5	Power input to stirred tank fermenters in practice
SuperPro Designer (2004)	3	Total Fermentation Operation (Batch Stoictiometric)

Centrifugation

Source	Value, yeast (kWh/m3 feed)	Value, bacteria (kWh/m^3 feed)	Comments
Tutunjian (1985)		6.2	Bacteria harvesting, continuous disc-type centrifuge, 37 HP motor, water removal rate 5 m^3/h
Tutunjian (1985)	1.4		Yeast harvesting, continuous disc-type centrifuge, 37 HP motor, water removal rate 5 m^3/h
Steffens et al. (1999, 2000)	1.5		Kennyedy and Cabral, 1993, p.169
Kalk and Langlykke (1986)	2.3		Case study: intracellular protein production, continuous desludging disk centrifuges, 4 m^3/h
Bohlmann (2002)	0.7 - 1.5		Nozzle centrifuge 149 kW, bakers yeast, feed 100-200 m^3/hr concentrate 20-50 m^3/hr
Bohlmann (2002)	0.9-1.9		Nozzle centrifuge 149 kW, brewers yeast, feed 80-160 m^3/hr concentrate 10-40 m^3/hr
Bohlmann (2002)	1.0-1.5		Nozzle centrifuge 149 kW, single cell protein, feed 50-100 m^3/hr concentrate 10-20 m^3/hr
Bohlmann (2002)	1.2-2.5		Nozzle centrifuge 149 kW, alcohol yeast, feed 60-120 m^3/hr concentrate 12-15 m^3/hr
Bohlmann (2002)		7.4-9.3	Axial solid ejecting centrifuge 37 kW, extracellular enzymes- bacterial amylases, feed 4-5 m^3/hr
Bohlmann (2002)		7.4	Axial solid ejecting centrifuge 37 kW, steroids, feed 5 m^3/hr
Bohlmann (2002)		9.3-12.3	Axial solid ejecting centrifuge 37 kW, harvesting *E. coli,* feed 3-4 m^3/hr
Bohlmann (2002)		19-25	Axial solid ejecting centrifuge 37 kW, *E. coli* cell debris feed 1.5-2 m^3/hr

Drying

Source	Steam req. (kg steam/kg evap.)	Electricity req. (kWh/kg	Comments
Reisman (1988)	2.0- 2.4	0.1	Tower dryer, no heat recovery. Savings of up to 25% in heating requirement are possible.
Gerngross (1999)	2		Spray drying of polymer slurry to yield a powder.
Bartholomew and Reisman (1979)	3	0.1	Spray dryer (in case study)
IPTS (2003)	1.2 - 1.67		Drying of food, 2.5-3.5MJ/kg
Energy Centre Denmark (1992)			Spray drying of food
	2.33		1 stage, 4.9 MJ/kg
	2.05		2 stages, 4.3 MJ/kg
	1.62		multistage, 3.4 MJ/kg
IPTS (2003)		0.25 - 1	Low temperature drying of food using a heat pump
IPTS (2003)	1.76		3.7 MJth/kg vapour. High temperature (about 600ºC) drying of sugar beet pulp in a co-current drum dryer using direct heating by flue gas. Evaporation of 46 t/h water.
IPTS (2003)	1.38		2.9 MJth/kg vapor. Two stage drying of sugar beet pulp. Low temperature (about 60ºC) drying in belt dryer using waste heat, followed by high temperature drying.
IPTS (2003)	0.24		0.5 MJth/kg vapor. Fluidized bed drying (convective) of sugar beet pulp. Superheated 25 bar steam is used in the evaporator to produce steam at 3 bar to be used as heating steam.
SuperPro Designer (2004)	*2*		*[see: Drying Operation: Utility Data Tab (Interface)]*

Electrodialysis

Source	Value	Comments
Novalic et al. (1995)	0.11 – 0.13	Separation of citric acid using bipolar membranes (excluding pumping). Dilute stream concentrations in the range of 5-20% have no significant influence on mass transfer.
Kim and Moon (2001)	0.11, 0.34, 0.13	(with different membranes) One stage, three-compartment water splitting ED of lactic acid, current efficiency ~80%, recovery >96%
Kim and Moon (2001)	0.07-0.087	Two-stage (desalting + WSED) ED of LA, with ion exchange. Current efficiency >80%, recovery 99%
Kim and Moon (2001)	0.09	Nanofiltration and one stage water splitting ED of LA, recovery 96%
Bohlmann (2002)	0.08	Succinic acid, electricity requirement including pumping for two-stage ED

Evaporation

Source	Steam req. (kg steam/kg evap.)	Electricity (kWh/kg	Comments
Seider et al. (1998)	1.25		Heuristic. Interstage steam pressures can be boosted with steam jet compressors of 20-30% efficiency or with mechanical compressors of 70-75% efficiency.
Lavis (1996)	1.1		Single-effect evaporator example
IPTS (2003)	1.2-1.4		Single stage evaporator in the food industry
Brocklebank (1990)	0.7		Two-stage evaporator
Gerngross (1999)	0.25		Triple-effect evaporator, concentrating a slurry from 30% to 50% solids.
Lavis (1996)	0.4		Triple-effect evaporator example
Lavis (1996)	0.3		Triple-effect evaporator with thermocompressor example
Brocklebank (1990)	0.2		Five-stage evaporator
IPTS (2003)	0.1-0.3	0.002	Multistage thermal vapor recompression in the food industry
Lavis (1996)	0.005	0.04	Single-effect mechanical vapor recompression example. 0.04kWh/kg (eq. 0.07 kg steam/kg)
IPTS (2003)		0.01	Mechanical vapor recompression in the food industry
Brocklebank (1990)	0.14	0.013	Five-stage mechanical compression system evaporating water boiling at 100 to 102ºC
Reisman (1988)	0.2		
Lo (1996)	0.4		Solvent recovery (toluene) in extraction plant
Schweitzer (nd), p.2-138			Feed rate: 25000 lb/h aqueous solution
	0.92	0.0035	First Effect, none recompression, 22891 lb steam /h, 40 kW
	0.32	0.0049	Thrid Effect, no recompression, 7997 lb steam/h, 55 kW
	0.27	0.0053	Thrid Effect,TVR recompression, 6649 lb steam/h, 60kW
	0.01	0.0344	First Effect, MVR recompression, 300 lb steam/h, 390 kW
SuperPro Designer (2004)	1.0764		Average Heat of Vaporisation is 540 kcal/kg vapor stream Batch evaporation (also known as single-stage batch distillation)

Appendix 5: Waste management

A5-1: Wastewater treatment

	Municipal wastewater					Distillery wastewater	Corn wetmill wastewater	Ethanol plant wastewater	**Biotech processes**
Source	Pers. comm., P. van der Pijl, TAUW, Feb. 2004	Pers. comm., R. J. Saft, IVAM, Feb.2004 (Case 1)[1)]	Pers. comm., R. J. Saft, IVAM, Feb.2004 (Case 2)[1)]	Owen, 1984 (Case 1)[2)]	Owen, 1984 (Case 2)[3)]	Ripley (1979)	Vink (2004)	Aden et al. (2002)[4) 5)]	**UU, CHOSEN FOR BREW**
COD/BOD	2.5	2.5	2.5	n.a.	n.a.	Assumed: 1.0	Assumed: 1.4 - 2.5	1.4	**1.0 - 2.5**
Primary energy use, MJ/kg COD	9.3	61.1	21.7	5.5	28 (16-41)	9.3	5.2 - 9.1	1.9	**7.5**

[1)] Case 1 is based on older but rather representative data. Case 2 is based on recent data but represents a specific case which may not be representative.

[2)] Referred to as a typical 30 t per day activated sludge plant with anaerobic digestion; the value quoted accounts for credits from digester gas (data from Owen, 1994, p.31).

[3)] Data for various treatment schemes (data from Owen, 1994, p.66). The value for the activated sludge plant with anaerobic digestion is 24 MJ/kg COD and is hence clearly higher than according to Case 1. Around 3.5 MJ/kg COD may be ascribed to unaccounted energy credits from digester gas in Case 2 but a substantial unexplained gap still remains between Case 1 and Case 2.

[4)] The value acc. to Aden et al. (2002) is exceptionally low. Possible reasons for the difference are: i) Lower COD/BOD ratio which facilitates the treatment ii) the anaerobic stage needs little energy (municipal water probably is treated only by aerobic activated sludge treatment) iii) no sludge treatment is included since it is combusted.

[5)] The value reported for primary energy use excludes energy credits for digester gas. Including this energy credit (11.3 MJ/kg COD) leads to a value of -9.4 MJ/kg COD, i.e. the wastewater treatment plant is a net energy source.

A5-2: Incineration of biomass with energy recovery

The table below presents power and heat production from solid biomass in an ethanol plant (Isaac, 2004; derived from Aden et al, 2002).

IN			OUT		
Distillation bottoms (to evaporator)	1	t dm	Net power output	2.69	GJ_{el}
Digestor solids (direct to combustor)	0.004	t dm	Net HP steam output	2.02	GJ_{th}
Biogas[1]	0.47	GJ	Net LP steam output	3.808	GJ_{th}
Compressed air	119	m_N3	Water from evaporator[3]	7.21	t
Make-up water	1.41	t	Wastewater	0.76	t
Heat for evaporation[2]	2.66	GJ	Ash	0.12	t

[1] Excluding small amounts of natural gas for startup

[2] Value for 3 effects and aqueous suspension with 10% solids (5.8% insoluble, 4.2% soluble). Depending on the process design the energy requirements for evaporation may be covered by waste heat (in this case waste heat from the distilllation column is used).

[3] Reused in the process

Based on the table above a dataset was developed for energy co-production from solid biomass in a White Biotechnology plant.

Input and outputs for heat recovery from biomass in an integrated CHP plant

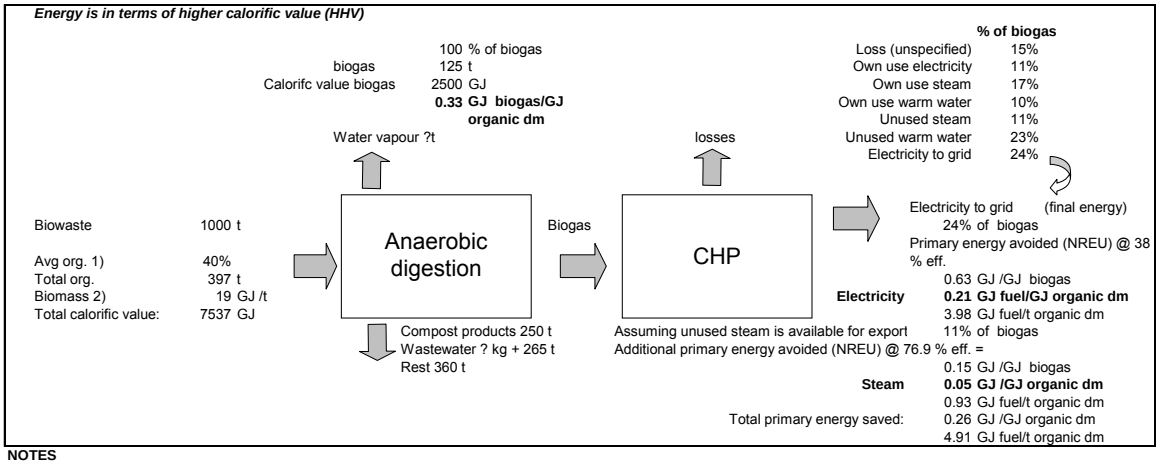
IN		OUT			
		Avoided primary energy (GJ HHV)		Avoided CO_2 emissions (t)	Avoided cost (EUR)
Biomass 1 t dm	19 GJ	Net power output	8.1 GJ primary	0.31 t	40.81
		Net steam output	7.6 GJ primary	0.47 t	33.30
Total input	1 t dm	per t dm input	15.6 GJ/t dm	0.78 t/t dm	74.11 EUR/t dm
	19 GJ	**per GJ input**	**0.82 GJ/GJ**	**0.041 t/GJ**	**3.90 EUR/GJ**

Assumptions for table above:

In	**Out**	**CO_2 emissions**	**Cost**
1 t distillation bottoms = 1 t biomass	Grid electricity generation = 33.4%	0.116 t CO_2/GJe (grid electricity)	15.17 EUR/Gje
Digestor solids neglected	steam raising efficiency = 76.9%	0.062 t CO_2/GJ fuel used for steam	12 EUR/t steam, 2.1 GJ/t
Biogas neglected			
Compressed air neglected	(Heat content of) water from evaporator neglected		

A5-3: Anaerobic digestion of biomass with energy recovery

Vagron plant, Groningen, the Netherlands a) p.100



NOTES

1) Organic dry matter is average for GFT from b).
2) HHV for biomass assumed to be 19 MJ HHV/kg organic dry matter.
3) From c): organic waste is GFT. The biowaste above refers to the organic wet fraction (OWF). Assume same composition of OWF as calculated from d).

SOURCES

a) De Mes, T.Z.D., Stams, A.J.M., Reith, J.H. and Zeeman, G (2003): Methane production by anaerobic digestion of wastewater and solid wastes, in: Reith, J.H., Wijffels, R.H., Barten, H. (eds): Bio-methane and Bio-hydrogen - Status and Perspectives of biological methane and hydrogen production. Dutch Biological Hydrogen Foundation 200, c/o ECN,
b) Provincie Antwerpen (1999): Onderzoek naar de mogelijke toepassing van nieuwe afvalverwerkingstekniеken in de provincie Antwerpen. Eindrapport. http://www.gomesanet.be/nederlands/publicaties/afvalsverwerking/19mei99.pdf
c) Vagron (2004): http://www.vagron.nl/html/uk/vagron4.htm
d) Brinkman and Schultz, 1997; cited in a) p.77.

Appendix 6: Sugar prices

Table A6-1: Prices of sugar from sugarcane (reproduction with kind permission from Tim Nisbet, Shell) L:\BioBasedMat_Lit\feedstocks\sugars\Sugar_price\ Updated Sugar Price.xls, sheet "Sugarcane"

Country	Year	Price $/t dry cane	Price $/t sugar	Reference
Brazil	1990	10.08	72 [1)]	C&T Brasil (2001)
Brazil	1999-00	9.55	68	ASSOCANA (2001)
Thailand	1997-98	13.98	100 [2)]	Thailand - Office of Agricultural Economics (2001)
	1999-00	11.42	82 [2)]	Thailand - Office of Agricultural Economics (2001)
South Africa	1998-99	21.58	154	South African Sugar Association
	1999-00	18.58	133	South African Sugar Association
	2000-01	19.58	166	South African Sugar Association
	2001-02	24.03	203	South African Sugar Association
	2002-03	25.68	210	South African Sugar Association
United States	1997	25.42	182 [3)]	US Department of Commerce (1999)
United States	1992	34.16	244 [3)]	US Department of Commerce (1999)
United States (Hawaii)	1995-97	21.25 [4)]	152 [5)]	Kinoshita and Zhou (1999)

Prices were converted from local currency to US dollars using the exchange rate for the reported year.

[1)] Feedstock cost for Ethanol production; estimate based on 0.45 t Ethanol/t sugar.

[2)] National average.

[3)] Sugarcane used for milling in the US.

[4)] Price reported was for dry cane; converted to wet (raw) cane using factor 0.25 MT dry cane/MT wet cane (Pate et al., 2001). A factor of 0.14 t sugar/t cane was used to calculate prices (Kinoshita and Zhou, 1999).

[5)] Estimate of sugarcane price (not delivered).

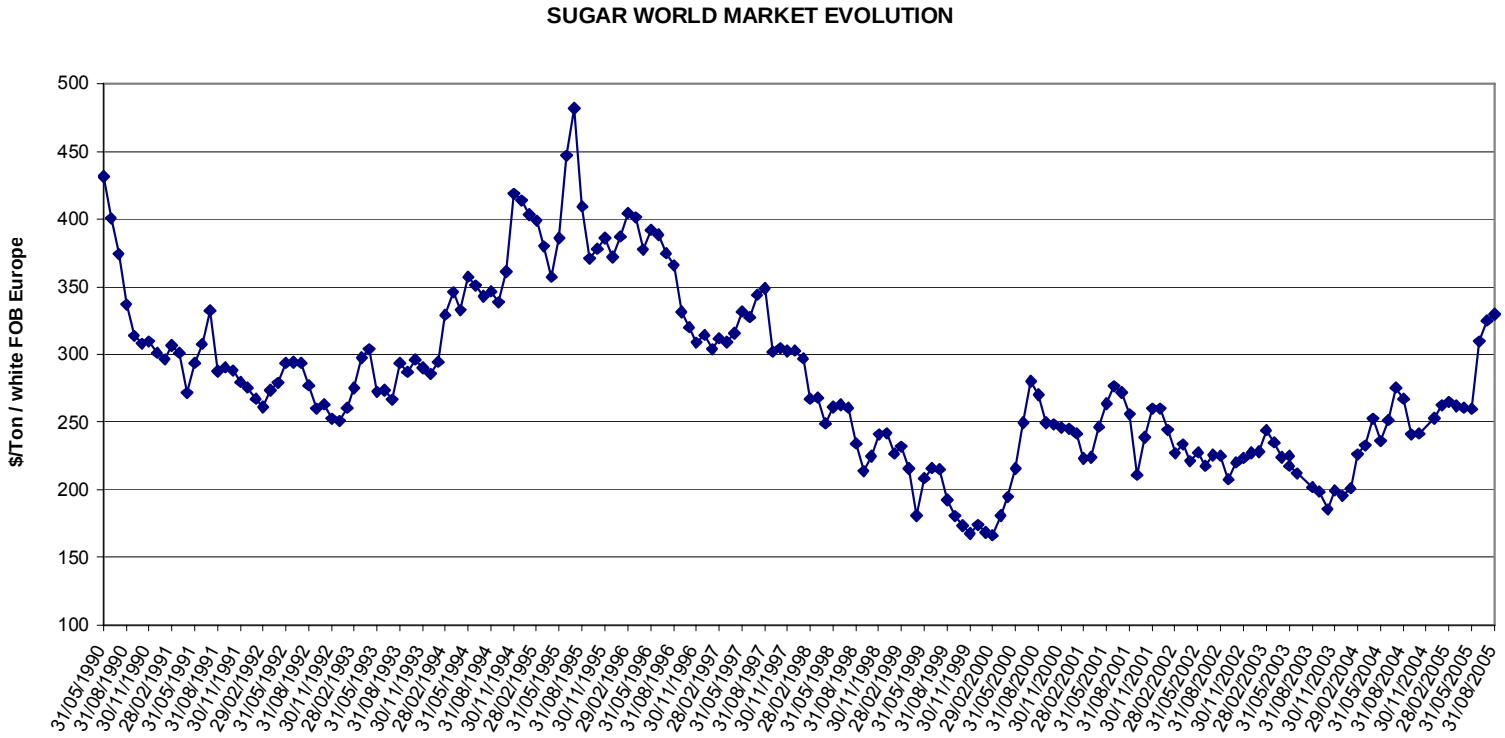


Figure A6-1: Development of the world market price for sugar 1990-2005 (F.I.R.S. 2005)

Appendix 7: Introduction to BREWtool

A7-1: BREWtool structure and file linkage

The structure and linkage of files for the BREWtool is shown schematically in Fig A7.1. The Excel file **BREWData.xls** contains all non-process-specific background data used in BREWtool calculations. Sheet **[FF]** (feedstocks and fuels) contains environmental impact data for 'second order' processes relating to the production of both non-renewable and renewable feedstocks, auxiliaries, catalysts, utilities and fuels. Data for bulk chemical intermediates and products (e.g., results of a BREWtool calculation or life cycle impacts reported in other sources) may also be stored here in the same format. Sheet **[UTIL]** (utilities) contains energy efficiency conversion factors and EU average data for electricity, steam and other utilities. Sheet **[ERE]** (energy requirements for energy) contains data relating to the extraction and primary processing of fossil mass to produce various types of non-renewable energy. Calculations in **[FF]** contain links to **[UTIL]** and **[ERE],** but not vice versa.
Process-specific background data are stored in a number of files together with literature references. In the product calculation sheet (file ***Productname*.xls**, sheet **[*Productname1*]**), process-specific background data is entered together with both the original literature reference (including page number) and, where relevant, the Excel file pathname (including cell reference). For non-process-specific data, data transfer to the product calculation sheet occurs via lookup functions. The product calculation sheet is thus linked to the file **BREWData.xls** sheet **[FF].** It is not linked to any other sheets.

A7-2: Structure of the Product Calculation Sheet

A separate Excel file is saved for each product. Within this file there are a number of calculation sheets, each being for a different production system leading to equivalent products. Each sheet has a fixed structure as explained below. Sections where data needs to be entered are in yellow.

Input

- Table of basic input data
- List of references
- Process flow scheme (block diagram)

Calculation

- Table(s) of process inputs/outputs – one table per sub-process; level of detail depends on the level of aggregation of available data (could be one process or several processes)
- Table(s) of background data for each input/output (environmental impacts associated with the production of each input/output). This data is automatically looked up from the file *BREWdata.*

- Table of results, automatically calculated according to input/output category

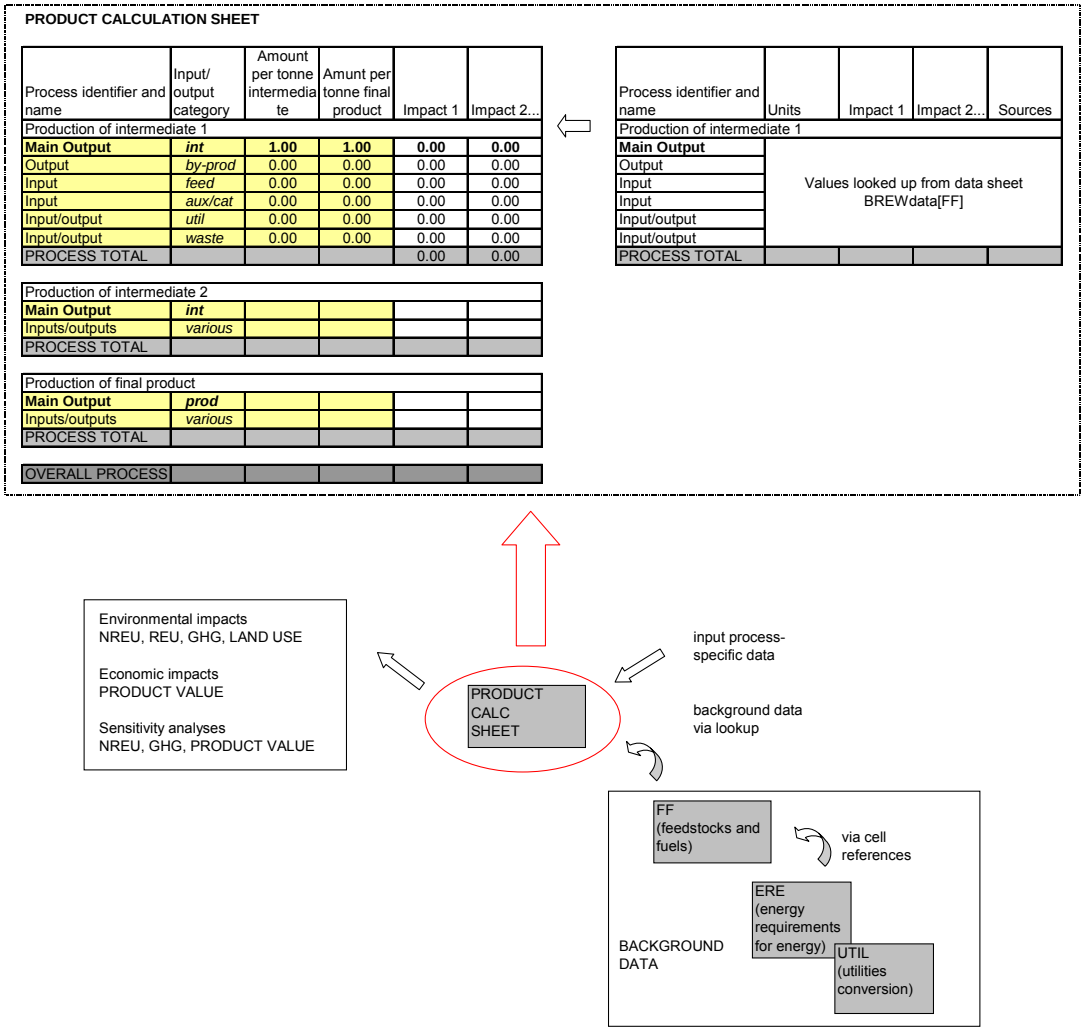


Fig A7.1 Schematic of BREWtool file structure

Results - Environmental Analysis

Table 1 shows the energy use (NREU, REU and TOTAL); GHG emissions (NREU, REU and TOTAL) according to four system boundaries:

- Cradle to factory gate
- Cradle to grave with impact-neutral waste management (no energy or material credits or debits for the waste management step)
- Cradle to grave, post-consumer waste management by digestion with energy recovery
- Cradle to grave, post-consumer waste management by incineration with energy recovery

Table 1 also shows land use for a cradle-to-factory gate system boundary.

Table 2 (and **Figure 1**) gives a breakdown of NREU and total GHG emissions by main input/output categories.

Table 3 (and **Figure 2**) gives a breakdown of NREU and total GHG emissions by user-defined categories. Default categories are: Substrate, Bioprocess (biotechnological process), Downstream (downstream processing/workup).

Results - Economic Analysis

Table 4 gives a breakdown of raw material and utility costs by main input/output categories.
Table 5 shows the calculation of production cost and product value according to the methodology outlined in Section xxx
Table 6 (and **Figure 3**) gives a breakdown of product value by various cost categories.

Results - Sensitivity Analysis

Table 7 (and **Figures 4 to 6**) show sensitivity analyses on NREU, GHG emissions and product value.

Results - Energy recovery Analysis

Tables 8 and 9 (and **Figures 7 and 8**) allow for comparison of NREU and GHG emissions for different post-consumer waste management options. Each option corresponds to a point on the sliding scale from *no (0%) energy recovery* to *ideal (100%) energy recovery*; generally lying between approximately 30% to 50% of ideal. Waste management with no energy recovery results in the highest NREU and GHG emissions; the higher the energy recovery the higher the reduction in NREU and GHG emissions due to avoided

A separate module in BREWtool is in charge of the scenario calculations.

Appendix 8: Abbreviations used to distinguish the processes studied with the Generic Approach and description of the processes

-ad	adsorption
-bat	batch process
-cont	continuous process
-c	crystallisation
-cat	catalyst
-cf	centrifugation
-d	distillation
-ev	evaporation
-ed	electrodialysis
-es	esterification
-ex	extraction
-ey	enzyme
-F	future
-gs	gas stripping
-h	homogenisation
-ix	ion exchange
-m	membrane separation
-n	neutralisation
-oa	oxidising agent
-P	past
-pv	pervaporation
-pc	precipitation
-rx	redox
-ro	reverse osmosis
-sp	spray drying
-T	today
-tes	transesterification
-u	unknown

The list of bio-based products which have been studied is shown in Table A10-1. Petrochemical processes serving as benchmarks are listed in Table A10-2. Processes are listed in alphabetical order according to the abbreviated name of the process, which will be used in subsequent sections for presentation of results. The prefix ‘bio’ is used to indicate that a product is produced partially or fully from biomass feedstock rather than from petrochemical feedstock. In cases where no commercially-viable bulk volume process based on petrochemical feedstock exists (e.g., lactic acid) the prefix ‘bio’ is not used with the bio-based product.

BIO-BASED PROCESSES

	Process abbreviation	Process description
Ethanol	BioEtOH-SRI-Td	Bio-ethanol via aerobic continuous fermentation on dextrose adapted from BioEtOH-SRI-Stover-Fd; workup via distillation
	BioEtOH-SRI-Corn-Td	Bio-ethanol via batch fermentation (enzyme, yeast) on corn starch; workup via distillation (SRI, 1982)
	BioEtOH-Anaer-GA-Tdcont	Bio-ethanol via anaerobic continuous fermentation on dextrose substrate; workup via distillation; Generic Approach (today)
	BioEtOH-Anaer-GA-Tpvcont	Bio-ethanol via anaerobic continuous fermentation on dextrose substrate; workup via pervaporation; Generic Approach (today)
	BioEtOH-Anaer-GA-Fd	Bio-ethanol via anaerobic continuous fermentation on dextrose substrate; workup via distillation; Generic Approach (future)
	BioEtOH-Anaer-GA-Fpv	Bio-ethanol via anaerobic continuous fermentation on dextrose substrate; workup via pervaporation; Generic Approach (future)
	BioEtOH-SRI-Stover-Fd	Bio-ethanol via aerobic continuous fermentation on corn stover (future technology); workup via distillation (SRI, 2003)
PDO	BioPDO-Aer-SRI-Tdcont	Bio-1,3-propanediol via aerobic continuous bioprocess on dextrose substrate, workup by evap/crystallisation and distillation (SRI, 1999).
	BioPDO-Anaer-SRI-Tdcont	Bio-1,3-propanediol via anaerobic continuous bioprocess on dextrose substrate, workup by evap/crystallisation and distillation (SRI, 1999).
	BioPDO-Aer-DP-Tu	Bio-1,3-propanediol via aerobic bioprocess on dextrose substrate; unspecified workup (DuPont, 2004).
	BioPDO-Aer-GA-Tevbat	Bio-1,3-propanediol via aerobic batch bioprocess on dextrose substrate, workup by evaporation and distillation, Generic Approach (today)
	BioPDO-Aer-GA-Tevcont	Bio-1,3-propanediol via aerobic continuous bioprocess on dextrose substrate, workup by evaporation and distillation, Generic Approach (today)
	BioPDO-Aer-GA-FpvH2O	Bio-1,3-propanediol via aerobic continuous bioprocess on dextrose substrate, workup by pervaporation of water, Generic Approach (future)
	BioPDO-Aer-GA-FpvPDO	Bio-1,3-propanediol via aerobic continuous bioprocess on dextrose substrate, workup by pervaporation of PDO, Generic Approach (future)
	BioPDO-Anaer-Glyc-SRI-Tdcont	Bio-1,3-propanediol via anaerobic continuous bioprocess on glycerol substrate, workup by evap/crystallisation and distillation (adapted from BioPDO-Anaer-SRI-Tdcont).
	BioPDO-Anaer-Glyc-VDI-Tdbat	Bio-1,3-propanediol via anaerobic batch bioprocess on glycerol substrate, workup by distillation (derived from Grothe, 2000).
ABE	BioABE-Anaer-GA-Tdcont	ABE via anaerobic continuous fermentation on dextrose substrate; workup via distillation; Generic Approach (today)
	BioABE-Anaer-GA-Tgscont	ABE via anaerobic continuous fermentation on dextrose substrate; workup via gas stripping; Generic Approach (today)
	BioABE-Anaer-GA-Fdm	ABE via anaerobic continuous fermentation on dextrose substrate; workup via distillation, membrane, distillation; Generic Approach (future)
	BioABE-Anaer-GA-Fmd	ABE via anaerobic continuous fermentation on dextrose substrate; workup via membrane, 2*distillation; Generic Approach (future)
	BioABE-Anaer-GA-Fpv	ABE via anaerobic continuous fermentation on dextrose substrate; workup via pervaporation; Generic Approach (future)
	BioABE-Anaer-GA-Fgs	ABE via anaerobic continuous fermentation on dextrose substrate; workup via gas stripping; Generic Approach (future)
Acetic acid	BioAcet-Anaer-GA-TexTOPO	Acetic acid via anaerobic batch fermentation on dextrose substrate; workup via extraction using TOPO; Generic Approach (today)
	BioAcet-Anaer-GA-Ted	Acetic acid via anaerobic batch fermentation on dextrose substrate; workup via electrodialysis; Generic Approach (today)
	BioAcet-Anaer-GA-FexTOPO	Acetic acid via anaerobic continuous fermentation on dextrose substrate; workup via extraction using TOPO; Generic Approach (future)
	BioAcet-Anaer-GA-FexDIPE	Acetic acid via anaerobic continuous fermentation on dextrose substrate; workup via extraction using diisopropylether; Generic Approach (future)
	BioAcet-Anaer-GA-FedexDIPE	Acetic acid via anaerobic continuous fermentation on dextrose substrate; workup via electrodialysis and extraction using diisopropylether; Generic Approach (future)
	BioAcet-Anaer-GA-Fed	Acetic acid via anaerobic continuous fermentation on dextrose substrate; workup via electrodialysis; Generic Approach (future)
Acrylic acid	BioAcryl-Anaer-GA-Fex	Bio-acrylic acid via anaerobic continuous fermentation on dextrose substrate; workup via extraction; Generic Approach (future)

Table A7-1: Bio-based processes based on company data or published literature

Lactic acid	BioLA-SRI-TpH6cont	Lactic acid via anaerobic, continuous pH6 fermentation by Lactobacillus delbrueckii on dextrose; workup via acidification and filtration. (SRI, 2001).
	BioLA-SRI-FlowpH	Lactic acid via anaerobic, continuous low pH fermentation by homolactic bacteria (CD) on dextrose; workup via extraction and distillation. (SRI, 2001).
	BioLA-NW-Tu	Lactic acid via anaerobic fermentation on dextrose; workup via unspecified process involving neutralisation & acidification. Nature Works process (NW, 2004a; Vink et al., 2004, 2004a); supplementary data from SRI process designs (SRI, 1996).
	BioLA-Sh-Fex	Lactic acid via anaerobic, continuous low pH fermentation on dextrose; workup via solvent extraction and distillation. Shell analysis based on BioLA-SRI-FlowpH process designs (Cano, 2001).
	BioLA-Sh-Fed	Lactic acid via anaerobic, continuous low pH fermentation on dextrose; workup via electrodialysis. Shell analysis based on BioLA-SRI-FlowpH process designs (Cano, 2001).
	BioLA-Anaer-GA-Fed	Lactic acid via anaerobic continuous fermentation on dextrose; workup via electrodialysis. Generic approach (future)
	BioLA-NW-Fu	Lactic acid via anaerobic fermentation on dextrose; workup via unspecified process involving neutralisation & acidification. Nature Works (NW, 2004a; Vink et al., 2004, 2004a); supplementary data from SRI process designs (SRI, 1996). Nature Works data
Succinic acid	BioSA-Anaer-GA-Tc	Bio-succinic acid via anaerobic batch fermentation on dextrose substrate; workup via crystallisation; Generic Approach (today)
	BioSA-Anaer-GA-Ted	Bio-succinic acid via anaerobic batch fermentation on dextrose substrate; workup via electrodialysis; Generic Approach (today)
	BioSA-Aer-SRI-Fed	Bio-succinic acid via aerobic continuous fermentation by Actinobacillus succinogenes 130Z on dextrose substrate; workup via electrodialysis (SRI, 2001).
	BioSA-Anaer-GA-Fcrx	Bio-succinic acid via anaerobic continuous fermentation on dextrose substrate; workup via crystallisation, equation is redox balanced; Generic Approach (future)
	BioSA-Anaer-GA-Fc	Bio-succinic acid via anaerobic continuous fermentation on dextrose substrate; workup via crystallisation; Generic Approach (future)
	BioSA-Anaer-GA-Fed	Bio-succinic acid via anaerobic continuous fermentation on dextrose substrate; workup via electrodialysis; Generic Approach (future)
Adipic acid	BioAdip-Aer-GA-Tc	Adipic acid via aerobic batch fermentation on dextrose substrate; workup via evaporation, crystallisation; Generic Approach (today)
	BioAdip-Aer-GA-Fc	Adipic acid via aerobic continuous fermentation on dextrose substrate; workup via evaporation, crystallisation; Generic Approach (future)
	BioAdip-Aer-GA-Fed	Adipic acid via aerobic continuous fermentation on dextrose substrate; workup via electrodialysis; Generic Approach (future)
Citric acid	BioCit-Aer-SRI-Tevc	Citric acid via aerobic fermentation on molasses substrate; workup via evaporation, crystallisation (SRI, 2002)
	BioCit-Aer-SRI-Tix	Citric acid via aerobic fermentation of dextrose substrate; workup via ion-exchange
	BioCit-Aer-GA-Tpc	Citric acid via aerobic batch fermentation on dextrose substrate; workup via precipitation; Generic Approach (today)
	BioCit-Aer-GA-Fc	Citric acid via aerobic continuous fermentation on dextrose substrate; workup via crystallisation; Generic Approach (future)
Caprolactam	BioCapro-Aer-GA-Fd	Bio-caprolactam via aerobic continuous fermentation to lysine on dextrose substrate; workup via distillation; Generic Approach (future)
Lysine	BioLys-Aer-SRI-Tix	Lysine*HCl via aerobic batch fermentation of C. glutamicum on dextrose substrate; workup via Ion Exchange; SRI, 2002
	BioLys-Aer-SRI-Tsp	Lysine-sulphate via aerobic batch fermentation of C. glutamicum on dextrose substrate; workup via spray drying (SRI, 1999)
	BioLys-Aer-GA-Tix	Bio-lysine via aerobic batch fermentation on dextrose substrate; workup via Ion Exchange; Generic Approach (today)
	BioLys-Aer-GA-Fad	Bio-lysine via aerobic continuous fermentation on dextrose substrate; workup via adsorption; Generic Approach (future)
Hydrogen	BioH2-A&F-gs	Bio-hydrogen from potato waste via hydrolysis to sugars followed by 2 stages of fermentation: 1st stage: thermophilic (dark) fermentation; 2nd stage: photo fermentation (A&F, 2003a; 2004a; 2004c; De Vrije and Claassen, 2003).

Table A8-1: Bio-based processes based on company data or published literature (cont'd.)

PHA	BioPHAmcl-A&F-D5:FA1-Tex	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation with unspecified microorganism on substrate of dextrose and fatty acid in the ratio 5:1 wt/wt; workup via solvent-free extraction (A&F, 2003; 2004; 2004b)
	BioPHAmcl-A&F-FA-Oilex	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation with p. putida on substrate fatty acid; workup via solvent-free extraction (A&F, 2003; 2004; 2004b)
	BioPHA-GA-Toa	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; workup via oxidising agent; Generic Approach (today)
	BioPHA-GA-Th	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; workup via homogenisation; Generic Approach (today)
	BioPHA-GA-Tey	Mid chain length poly(hydroxyalkanoate) via fermentation on dextrose; workup via enzymatic solubilisation; Generic Approach (today)
	BioPHA-GA-Tex	Mid chain length poly(hydroxyalkanoate) via fermentation on dextrose; workup via solvent extraction; Generic Approach (today)
	BioPHA-GA-Texey	Mid chain length poly(hydroxyalkanoate) via fermentation on dextrose; workup via enzymatic solubilisation and solvent extraction; Generic Approach (today)
	BioPHA-GA-OilTexey	Mid chain length poly(hydroxyalkanoate) via fermentation on rapeseed oil; workup via enzymatic solubilisation and solvent extraction; Generic Approach (today)
	BioPHBV-SRI-Tey-1	Mid chain length poly(hydroxyalkanoate) in latex form via continuous fermentation on dextrose; workup via enzymatic solubilisation; PEP Yearbook 2M-669
	BioPHB-SRI-Tey-2	Polyhydroxyvalerate via fermentation on dextrose; workup via enzymatic digestion; PEP Report 2002-8; contrary to the original source it is assumed in the BREW project that glucose is used instead of food waste as feedstock and as a consequence, a higher yield has been assumed.
	BioPHA-GA-Fey-1	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; workup via enzymatic solubilisation and centrifugation; Generic approach (future); data for auxiliaries (es. EDTA and SDS) have been estimated on the basis of de Koning, 1997
	BioPHA-GA-Fey-2	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; workup via enzymatic digestion; Generic approach (future); data for auxiliaries (es. EDTA and SDS) have been estimated on the basis of SRI report 2002-8 (polyhydroxyalkanoates from organic waste)
Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	Ethylene by dehydration of bioethanol acc. to Shell. Bioethanol via process BioEtOH-Anaer-GA-Tdcont
	BioEthylene-BioEtOH-Anae-GA-Fpv	Ethylene by dehydration of bioethanol acc. to Shell. Bioethanol via process BioEtOH-Anaer-GA-Fpv
Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	Ethyl lactate via pervaporation-assisted esterification of lactic acid on dextrose substrate. One step process; low pH fermentation of lactic acid (future); lactic acid is not isolated (Cano, 2001). Petrochemical ethanol, market price.
	EL-Sh-pchemEtOH-bioLA-F2	Ethyl lactate via pervaporation-assisted esterification of lactic acid on dextrose substrate. One step process; low pH fermentation of lactic acid (future); lactic acid is not isolated (Cano, 2001). Petrochemical ethanol, product value (PchemEtOH-Ethylene).
	BioEL-NW-bioEtOH-bioLA-T1	Fermentation to lactic acid (BioLA-NW-Tu), conversion to lactide, conversion to ethyl lactate (NatureWorks, 2005) with bio-ethanol (BioEtOH-Anaer-GA-Tdcont).
	BioEL-Sh-bioEtOH-bioLA-F3	Ethyl lactate via pervaporation-assisted esterification of lactic acid on dextrose substrate. One step process; low pH fermentation of lactic acid (future); lactic acid is not isolated (Cano, 2001). Bio-ethanol from corn.
	BioEL-Sh-bioEtOH-bioLA-F4	Ethyl lactate via pervaporation-assisted esterification of lactic acid on dextrose substrate. One step process; low pH fermentation of lactic acid (future); lactic acid is not isolated (Cano, 2001). Bio-Ethanol (BioEtOH-Anaer-GA-Tdcont).

Table A8-1: Bio-based processes based on company data or published literature (cont'd.)

PLA	BioPLA-bioLA-SRI-TpH6cont	Poly(lactic acid) via polycondensation of lactic acid (Nature Works, 2004, 2004b; Vink, 2003). Lactic acid via process BioLA-SRI-TpH6cont.
	BioPLA-bioLA-SRI-FlowpH	Poly(lactic acid) via polycondensation of lactic acid (Nature Works, 2004, 2004b; Vink, 2003). Lactic acid via process BioLA-SRI-FlowpH.
	BioPLA-bioLA-NW-Tu	Poly(lactic acid) via polycondensation of lactic acid (Nature Works, 2004, 2004b; Vink, 2003). Lactic acid via process BioLA-NW-Tu.
	BioPLA-bioLA-Sh-Fex	Poly(lactic acid) via polycondensation of lactic acid (Nature Works, 2004, 2004b; Vink, 2003). Lactic acid via process BioLA-Sh-Fex.
	BioPLA-bioLA-Sh-Fed	Poly(lactic acid) via polycondensation of lactic acid (Nature Works, 2004, 2004b; Vink, 2003). Lactic acid via process BioLA-Sh-Fed.
	BioPLA-bioLA-Anaer-GA-Fed	Poly(lactic acid) via polycondensation of lactic acid (Nature Works, 2004, 2004b; Vink, 2003). Lactic acid via process BioLA-Anaer-GA-Fed.
	BioPLA-bioLA-NW-Fu	Poly(lactic acid) via polycondensation of lactic acid (Nature Works, 2004, 2004b; Vink, 2003). Lactic acid via process BioLA-NW-Fu.
PTT	PTT-bioPDO-Aer-SRI-Tdcont	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Aer-SRI-Tdcont.
	PTT-bioPDO-Anaer-SRI-Tdcont	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Anaer-SRI-Tdcont.
	PTT-bioPDO-Aer-DP-Tu	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Aer-DP-Tu.
	PTT-bioPDO-Aer-GA-Tevbat	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Aer-GA-Tevbat.
	PTT-bioPDO-Aer-GA-Tevcont	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Aer-GA-Tevcont.
	PTT-bioPDO-Aer-GA-FpvH2O	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Aer-GA-FpvH2O.
	PTT-bioPDO-Aer-GA-FpvPDO	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Aer-GA-FpvPDO.
	PTT-bioPDO-Anaer-Glyc-SRI-Td	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Anaer-Glyc-SRI-Tdcont.
	PTT-bioPDO-Anaer-Glyc-VDI-Td	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid (SRI 1999). Bio-1,3-propanediol via process BioPDO-Anaer-Glyc-VDI-Tdbat.

Table A8-1: Bio-based processes based on company data or published literature (cont'd.)

PETROCHEMICAL-BASED PROCESSES

	Process abbreviation	Process description
Ethanol	PchemEtOH-1	Ethanol production from ethylene by catalytic hydration; based on SRI data
	PchemEtOH-2	Ethanol production from ethylene by catalytic hydration; based one project C-STREAMS (Patel et al, 1999).
PDO	PchemPDO-Propyl-DP	1,3-propanediol (PDO) via petrochemical process based on propylene, DuPont
	PchemPDO-EO-SRI	1,3-propanediol (PDO) via ethylene oxide (SRI, 1999). Ethylene oxide via ethylene (Chem Systems, 1998).
	PchemPDO-Acro-SRI	1,3-propanediol (PDO) via hydration of acrolein (SRI, 1999). Acrolein via oxidation of propylene.
ABE	PchemButanol	n-butanol from propylene via n-butyraldehyde, rhodium catalyst (PEP Yearbook, 2000)
Acetic acid	PchemAceticAcid	Acetic acid from ethylene via acetaldehyde (PEP Yearbook, 2000)
Acrylic acid	PchemAcrylicAcid	Acrylic acid from propylene by two-stage oxidation (PEP Yearbook, 2000)
Succinic acid	PchemSA-MalAnhydr	Succinic acid via catalytic hydrogenation of maleic anhydride (Ecoinvent, 2003). Maleic anhydride via partial oxidation of n-butane (Fumagalli, 1997)
	PchemMaleicAnhydr	Maleic anhydride via partial oxidation of n-butane (maleic acid as possible petrochemical equivalent of succinic acid)
Adipic acid	PchemAdipicAcid	Petrochemical adipic acid according to the C-STREAMS project (Patel et al. 1999)
Caprolactam	PchemCapro	Petrochemical caprolactam according to the C-STREAMS project (Patel et al. 1999)
H_2	PchemH2	Hydrogen from natural gas (estimate based on various sources)
Ethylene	PchemEthylene	Ethylene produced by steam cracking of naphtha according to APME
Solvents	PchemEthylAcetate	Petrochemical ethylacetate (various sources)
	PchemBenzene	Petrochemical benzene according to APME
	PchemEGBE	Petrochemical ethylene glycol butyl ether (EGBE; various sources)
	PchemMEK	Petrochemical ethyl methyl ketone (various sources)
	PchemAcetone	Petrochemical acetone according to the C-STREAMS project (Patel et al. 1999)
Polymers	PchemHDPE	High density polyethylene via polymerisation of ethylene (APME, 2003)
	PchemPE LD	Low density polyethylene via polymerisation of ethylene (APME, 2003)
	PchemPET Amorph	Amorphous poly(ethylene terephthalate) by polymerisation of ethylene and purified terephthalic acid (APME, 2003)
	PchemPS	General Purpose polystyrene by polymerisation of styrene (APME, 2003)
	PchemNylon-6	Petrochemical nylon 6 according to APME
	PchemNylon-6,6	Petrochemical nylon 6,6 according to APME
	PTT-PchemPDO-Propyl-DP	Poly(trimethylene terephthalate) via polycondensation of 1,3-propanediol and purified terephthalic acid (SRI 1999). 1,3-propanediol via process PchemPDO-Propyl-DP.
	PTT-PchemPDO-EO-SRI	Poly(trimethylene terephthalate) via polycondensation of 1,3-propanediol and purified terephthalic acid (SRI 1999). 1,3-propanediol via process 1,3-PchemPDO-EO-SRI.
	PTT-PchemPDO-Acro-SRI	Poly(trimethylene terephthalate) via polycondensation of 1,3-propanediol and purified terephthalic acid (SRI 1999). 1,3-propanediol via process PchemPDO-Acro-SRI.

Table A8-2: Petrochemical processes based on company data or published literature

Appendix 9: Process Flow Diagrams prepared for the Generic Approach

1. **Ethanol**
   - 1.1 BioEtOH-Anaer-GA-Tdcont
   - 1.2 BioEtOH-Anaer-GA-Fd
   - 1.3 BioEtOH-Anaer-GA-Fpv

2. **PDO**
   - 2.1 BioPDO-Aer-GA-Tevbat
   - 2.2 BioPDO-Aer-GA-Tevcont
   - 2.3 BioPDO-Aer-GA-FpvH2O
   - 2.4 BioPDO-Aer-GA-FpvPDO

3. **ABE**
   - 3.1 BioABE-Anaer-GA-Tdcont
   - 3.2 BioABE-Anaer-GA-Tgscont
   - 3.3 BioABE-Anaer-GA-Fdm
   - 3.4 BioABE-Anaer-GA-Fmd
   - 3.5 BioABE-Anaer-GA-Fpv
   - 3.6 BioABE-Anaer-GA-Fgs

4. **Acetic acid**
   - 4.1 BioAcet-Anaer-GA-TexTOPO
   - 4.2 BioAcet-Anaer-GA-Ted
   - 4.3 BioAcet-Anaer-GA-FexTOPO
   - 4.4 BioAcet-Anaer-GA-FexDIPE
   - 4.5 BioAcet-Anaer-GA-FedexDIPE
   - 4.6 BioAcet-Anaer-GA-Fed

5. **Acrylic acid**
   - 5.1 BioAcryl-Anaer-GA-Fex

6. **Lactic acid**
   - 6.1 BioLA-Anaer-GA-Fed

7. **Succinic acid**
   - 7.1 BioSA-Anaer-GA-Tc
   - 7.2 BioSA-Anaer-GA-Ted
   - 7.3 BioSA-Anaer-GA-Fcrx
   - 7.4 BioSA-Anaer-GA-Fc
   - 7.5 BioSA-Anaer-GA-Fed

8. **Adipic acid**
   - 8.1 BioAdip-Aer-GA-Tc
   - 8.2 BioAdip-Aer-GA-Fc
   - 8.3 BioAdip-Aer-GA-Fed

9. **Citric acid**
   - 9.1 BioCit-Aer-GA-Tpc
   - 9.2 BioCit-Aer-GA-Fc

10. **Caprolactam**
   - 10.1 BioCapro-Aer-GA-Fd

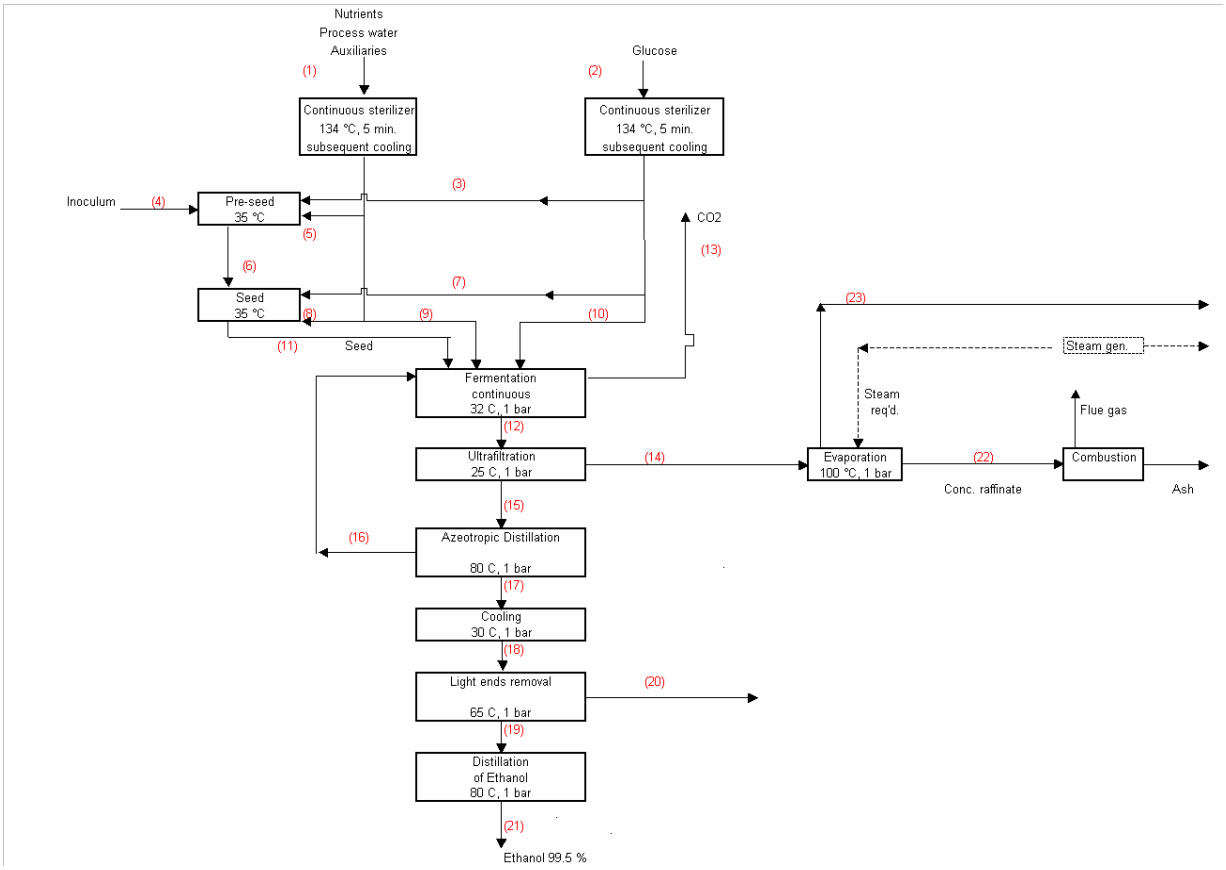
11. **Lysine**
   - 11.1 BioLys-Aer-GA-Tix
   - 11.2 BioLys-Aer-GA-Fad

12. **Hydrogen**
   - 12.1 BioH2-A&F-gs

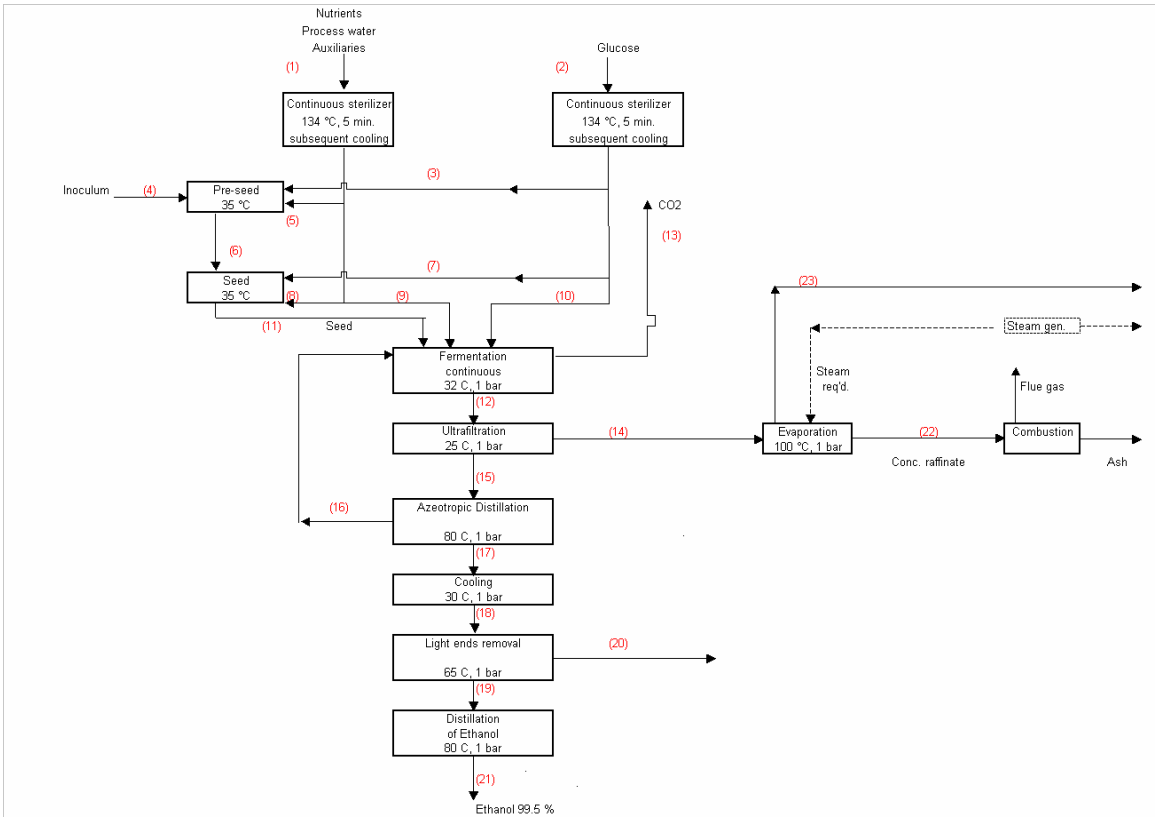
13. **PHA**
   - 13.1 BioPHA-GA-Toa
   - 13.2 BioPHA-GA-Th
   - 13.3 BioPHA-GA-Tey
   - 13.4 BioPHA-GA-Tex
   - 13.5 BioPHA-GA-Texey
   - 13.6 BioPHA-GA-OilTexey
   - 13.7 BioPHA-GA-Fey-1, BioPHA-GA-Fey-2

1. Ethanol

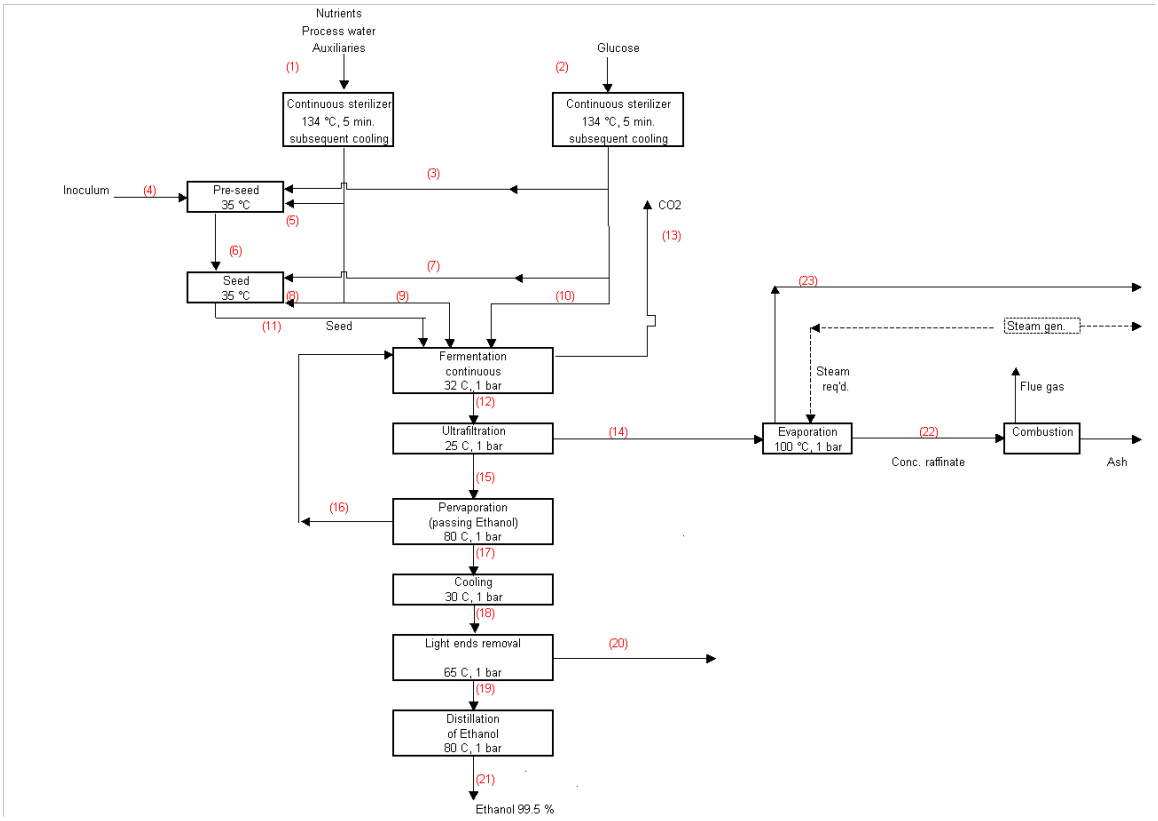
1.1 BioEtOH-Anaer-GA-Tdcont



1.2 BioEtOH-Anaer-GA-Fd

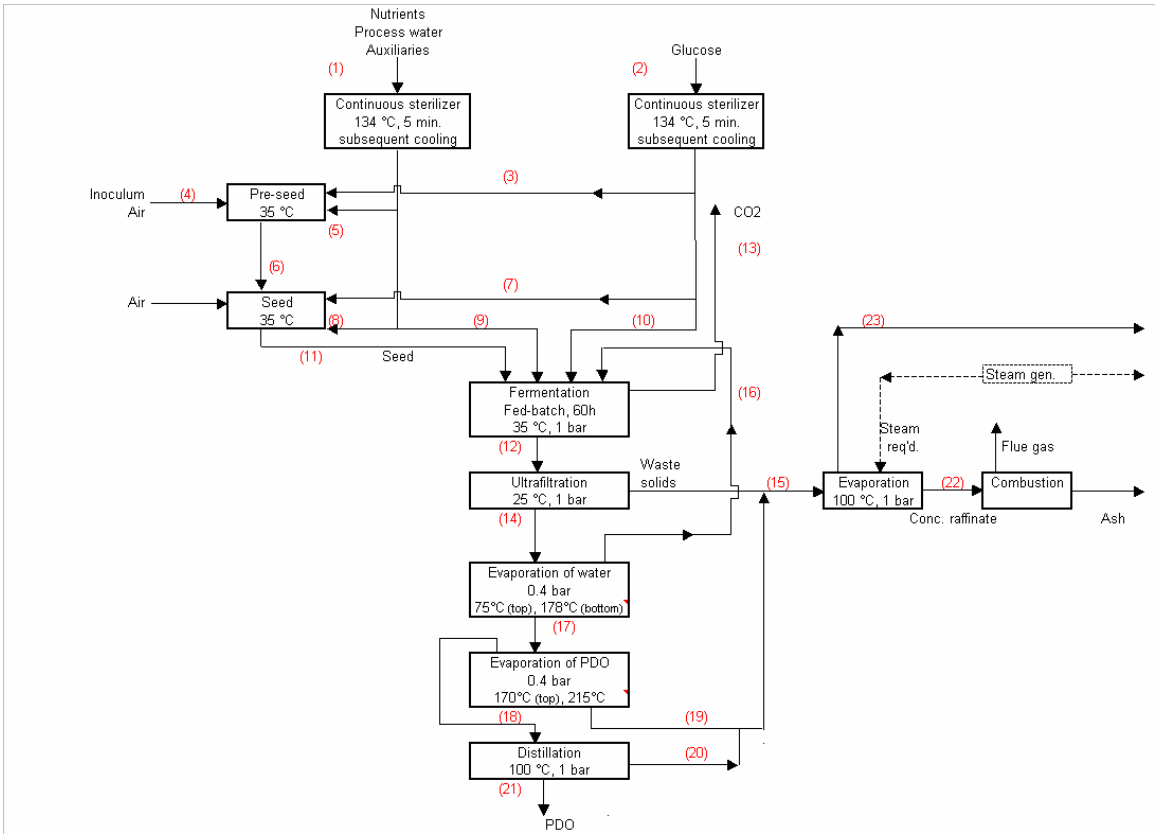


1.3 BioEtOH-Anaer-GA-Fpv

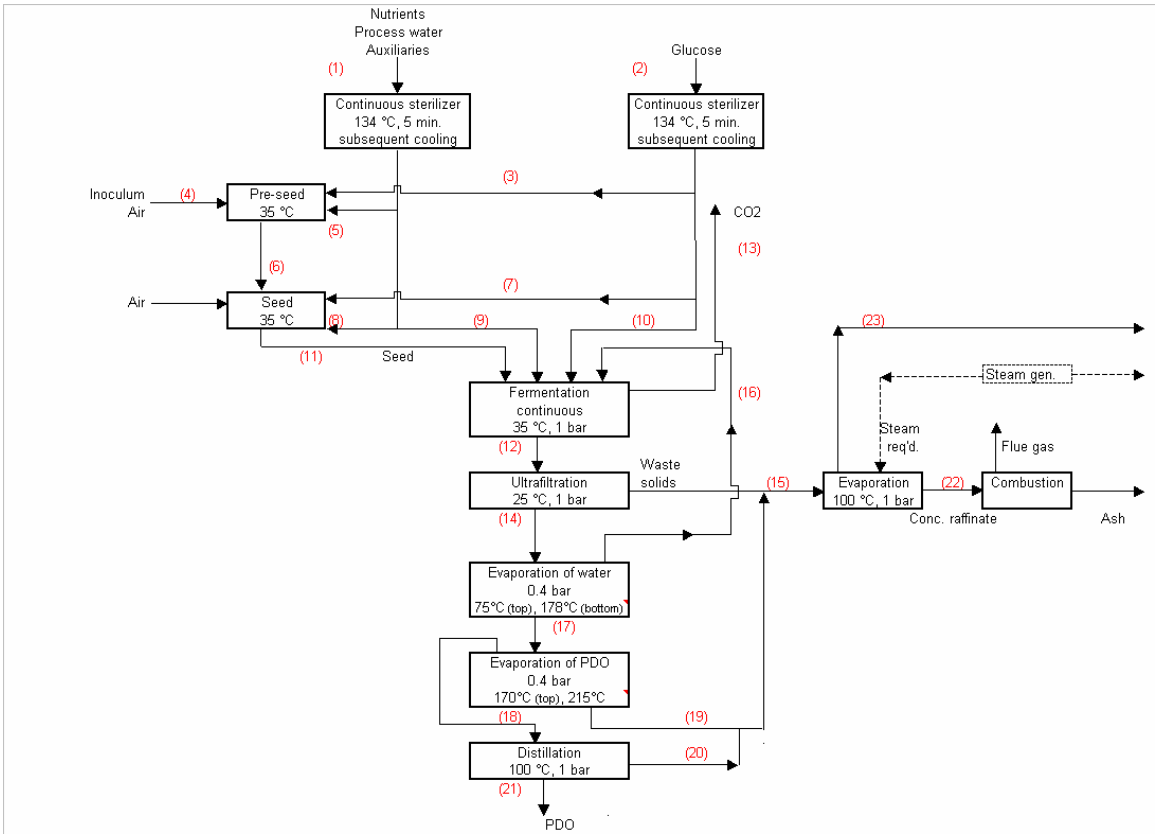


2. PDO

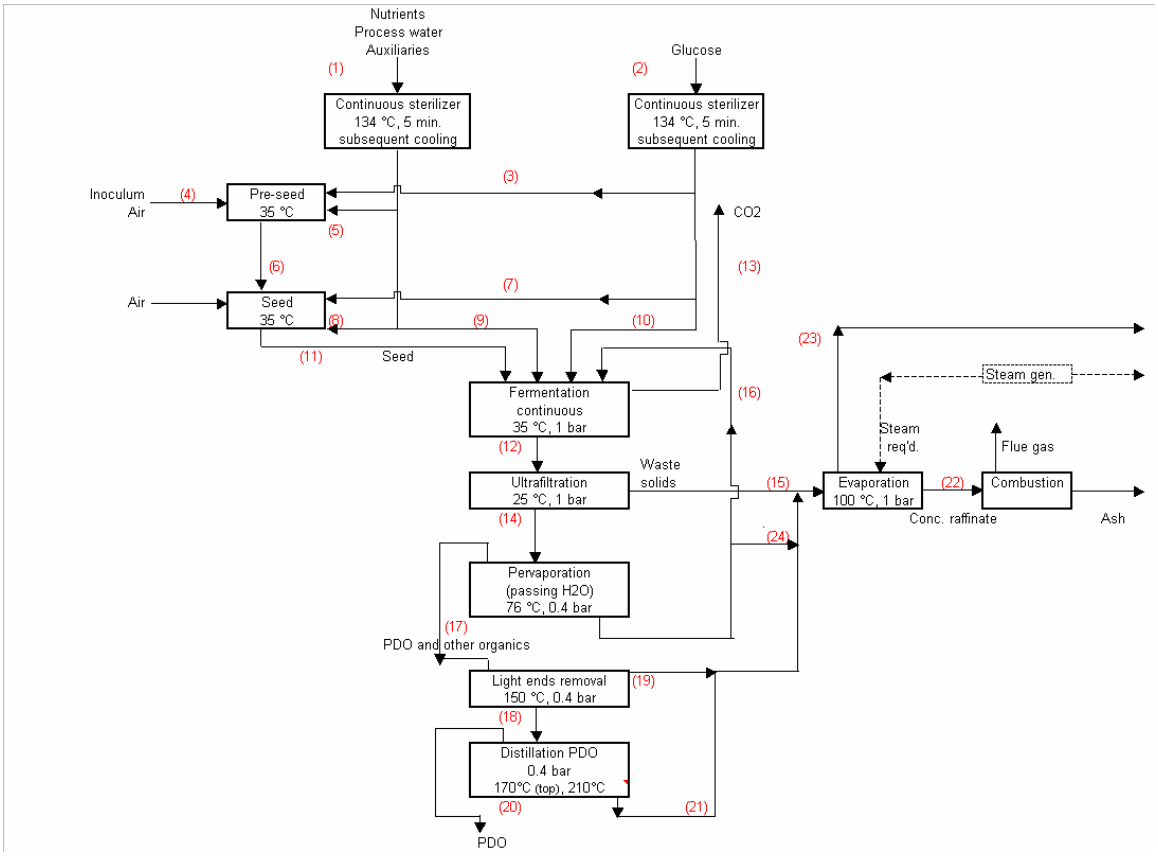
2.1 BioPDO-Aer-GA-Tevbat



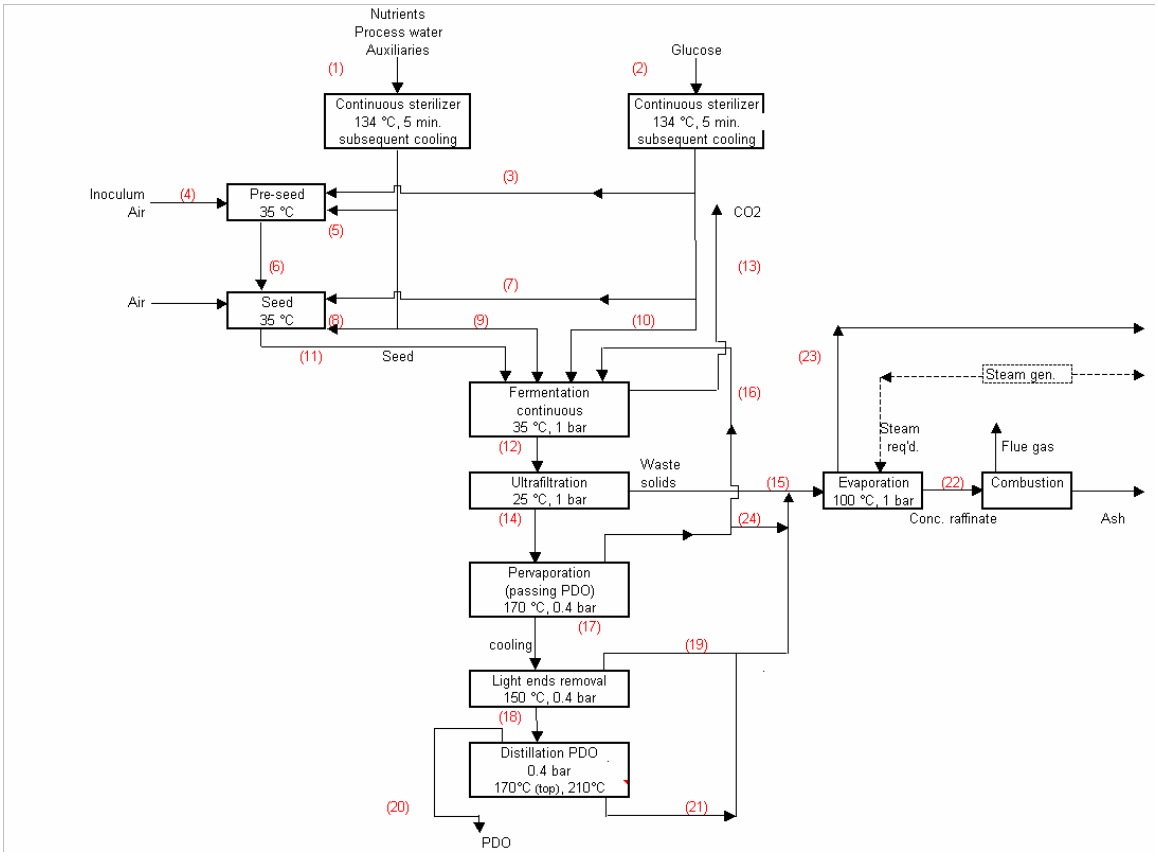
2.2 BioPDO-Aer-GA-Tevcont



2.3 BioPDO-Aer-GA-FpvH2O

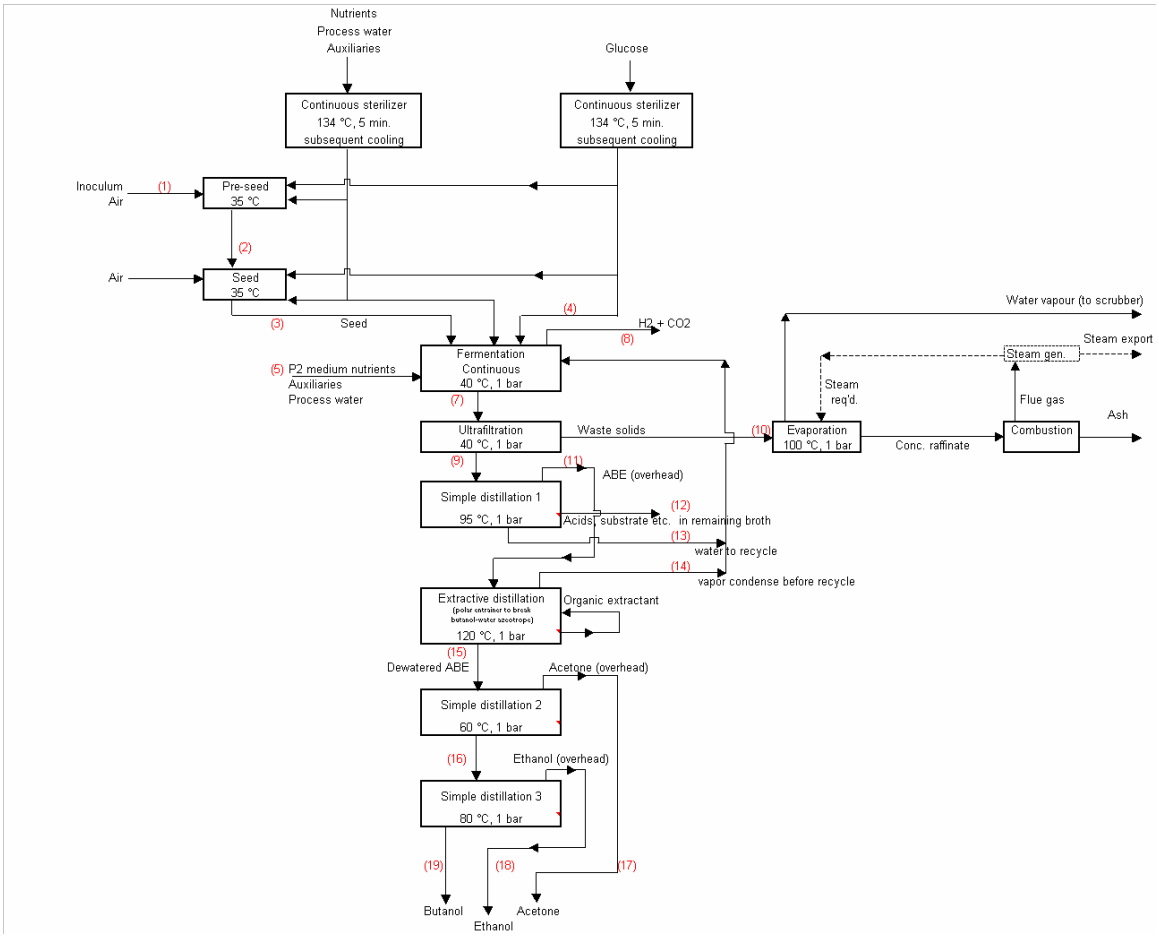


2.4 BioPDO-Aer-GA-FpvPDO

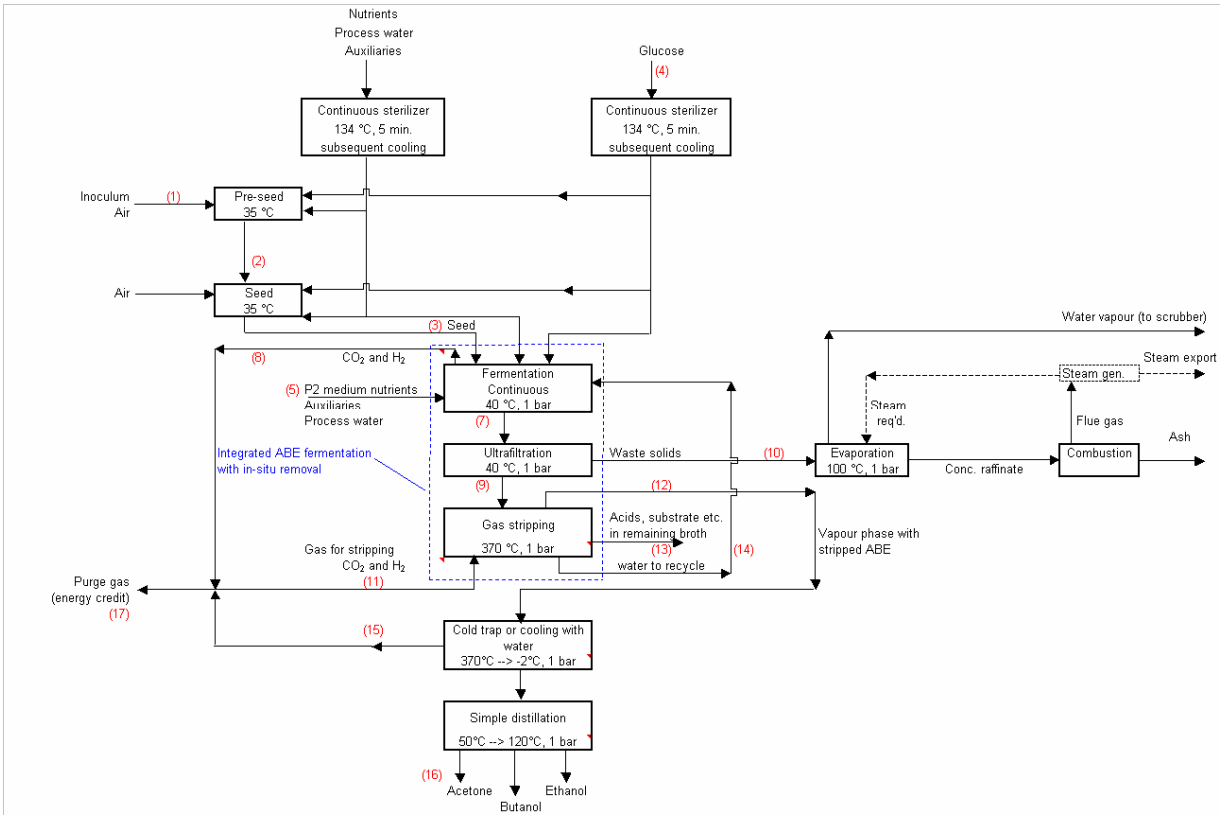


3. ABE

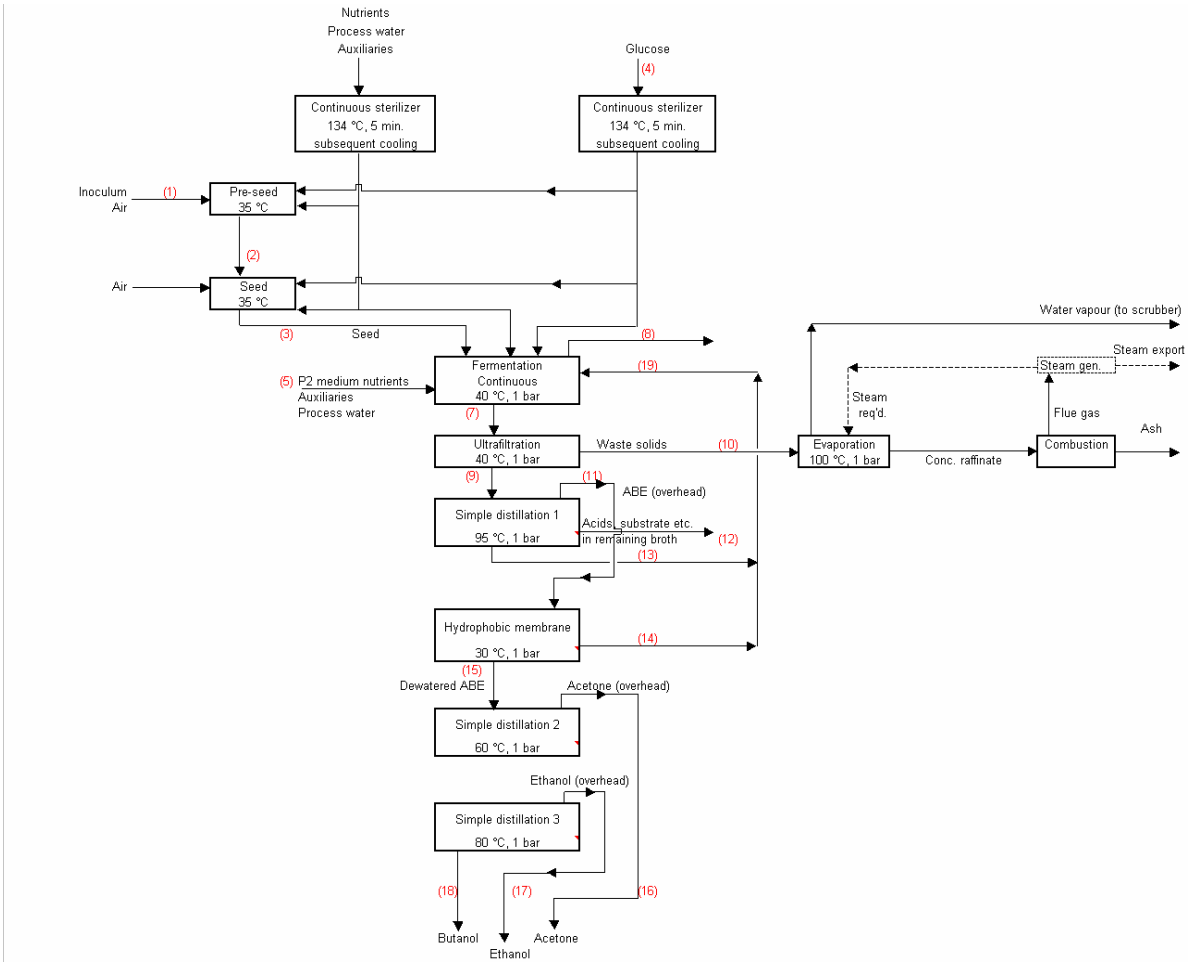
3.1 BioABE-Anaer-GA-Tdcont



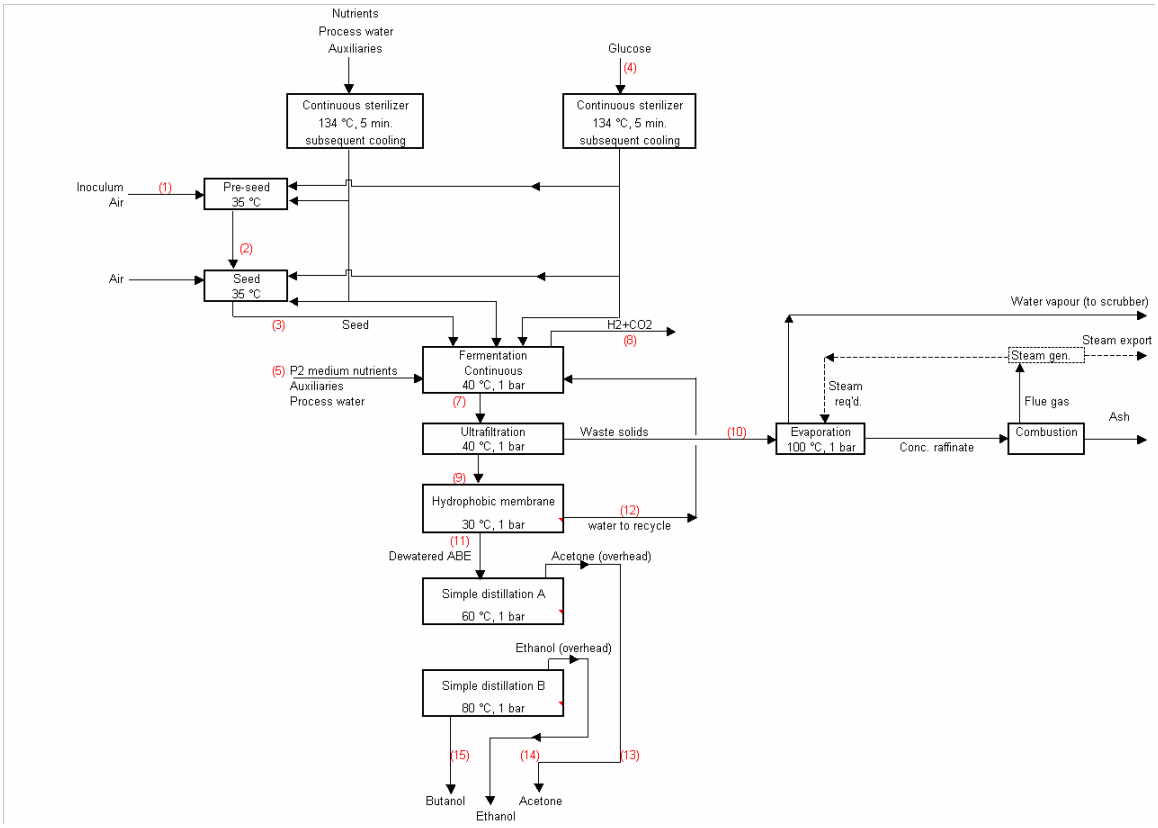
3.2 BioABE-Anaer-GA-Tgscont



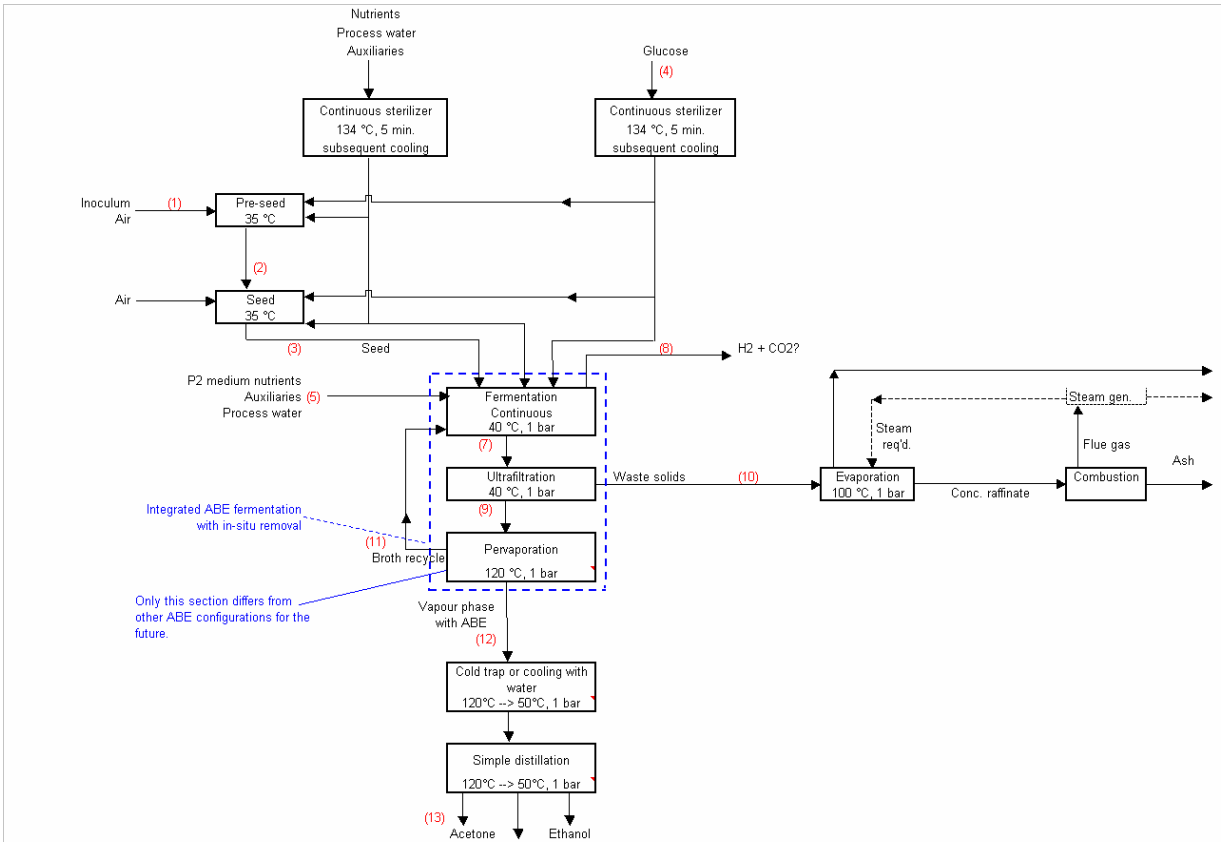
3.3 BioABE-Anaer-GA-Fdm



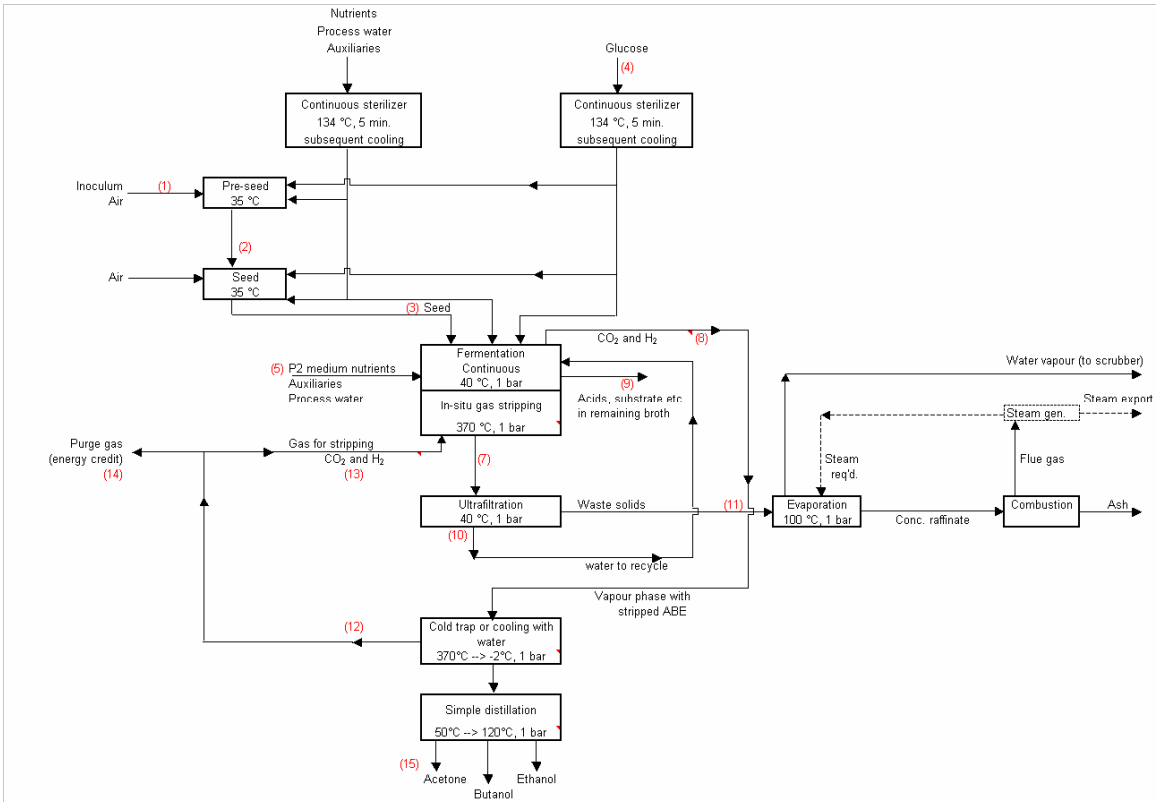
3.4 BioABE-Anaer-GA-Fmd



3.5 BioABE-Anaer-GA-Fpv

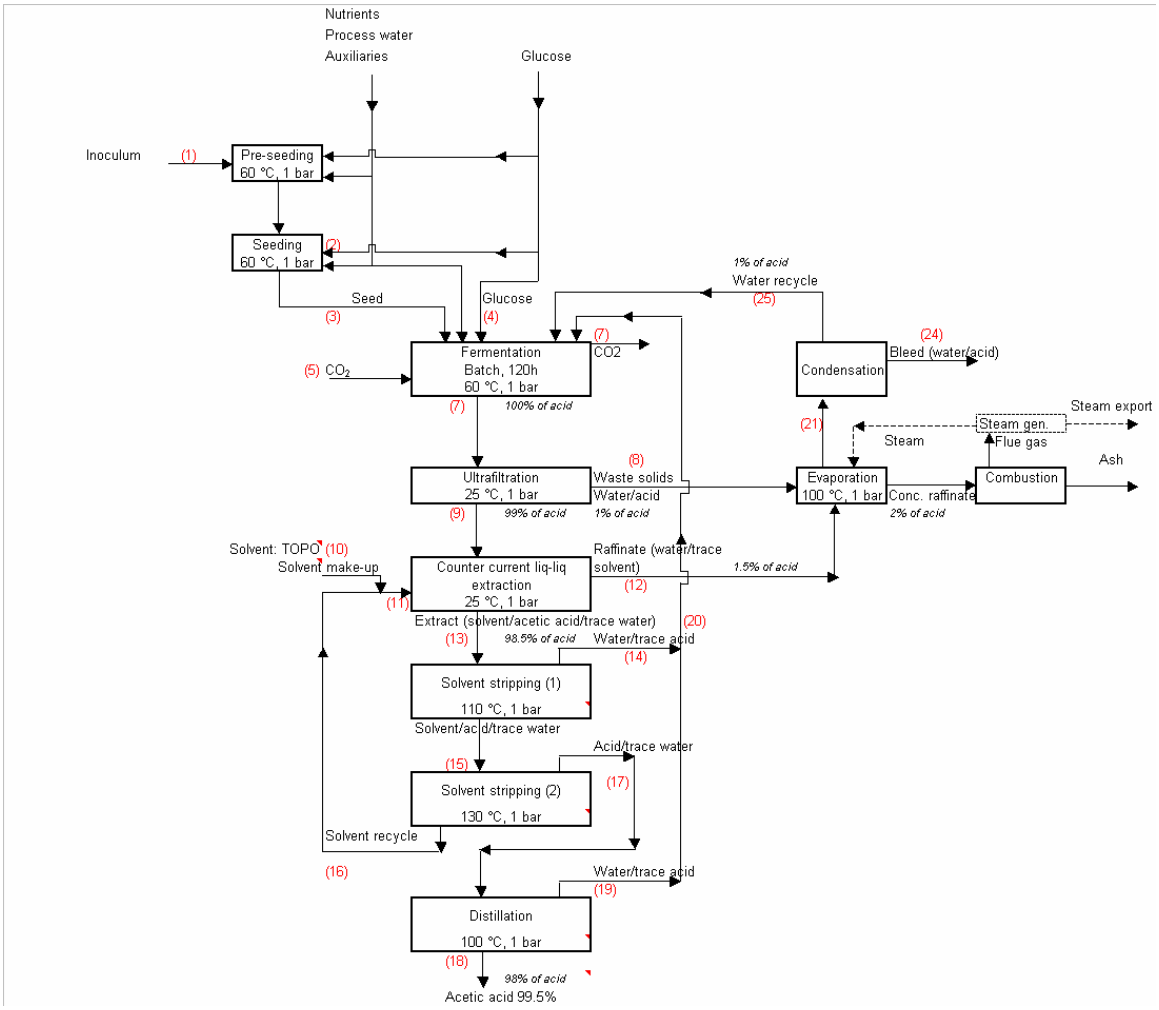


3.6 BioABE-Anaer-GA-Fgs

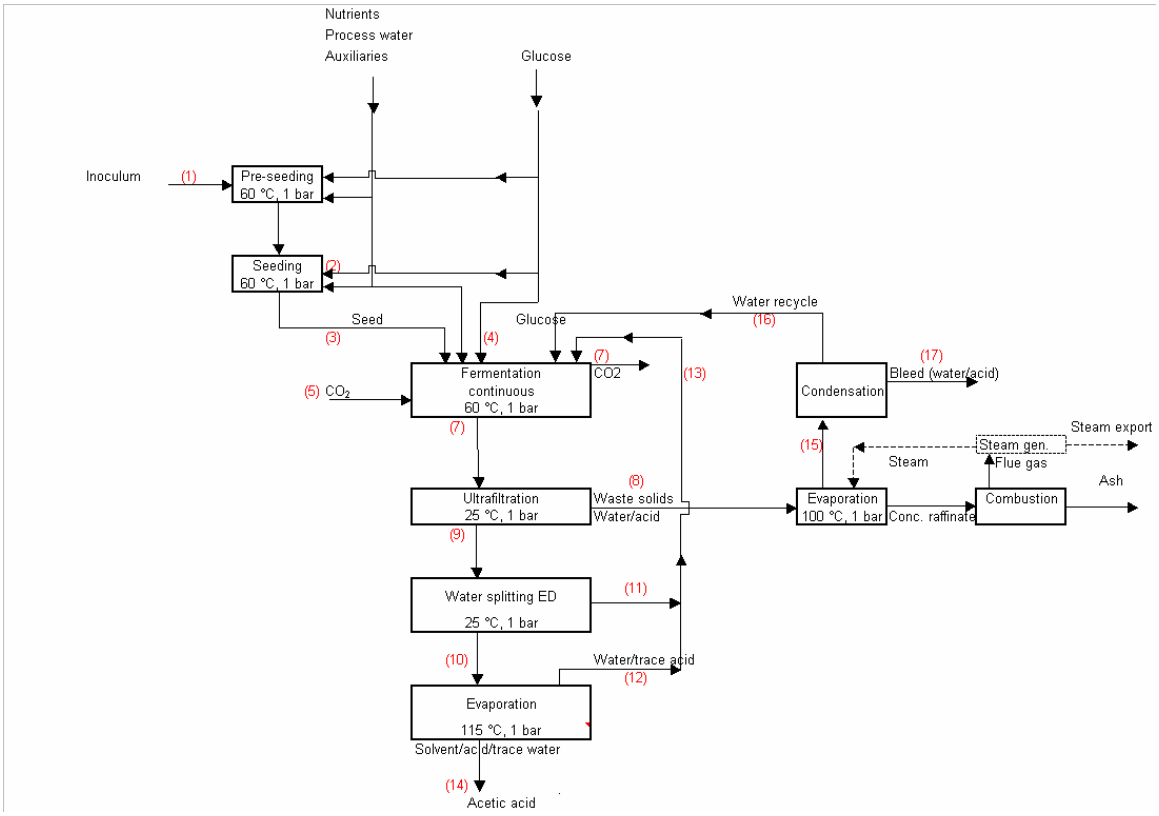


4. Acetic acid

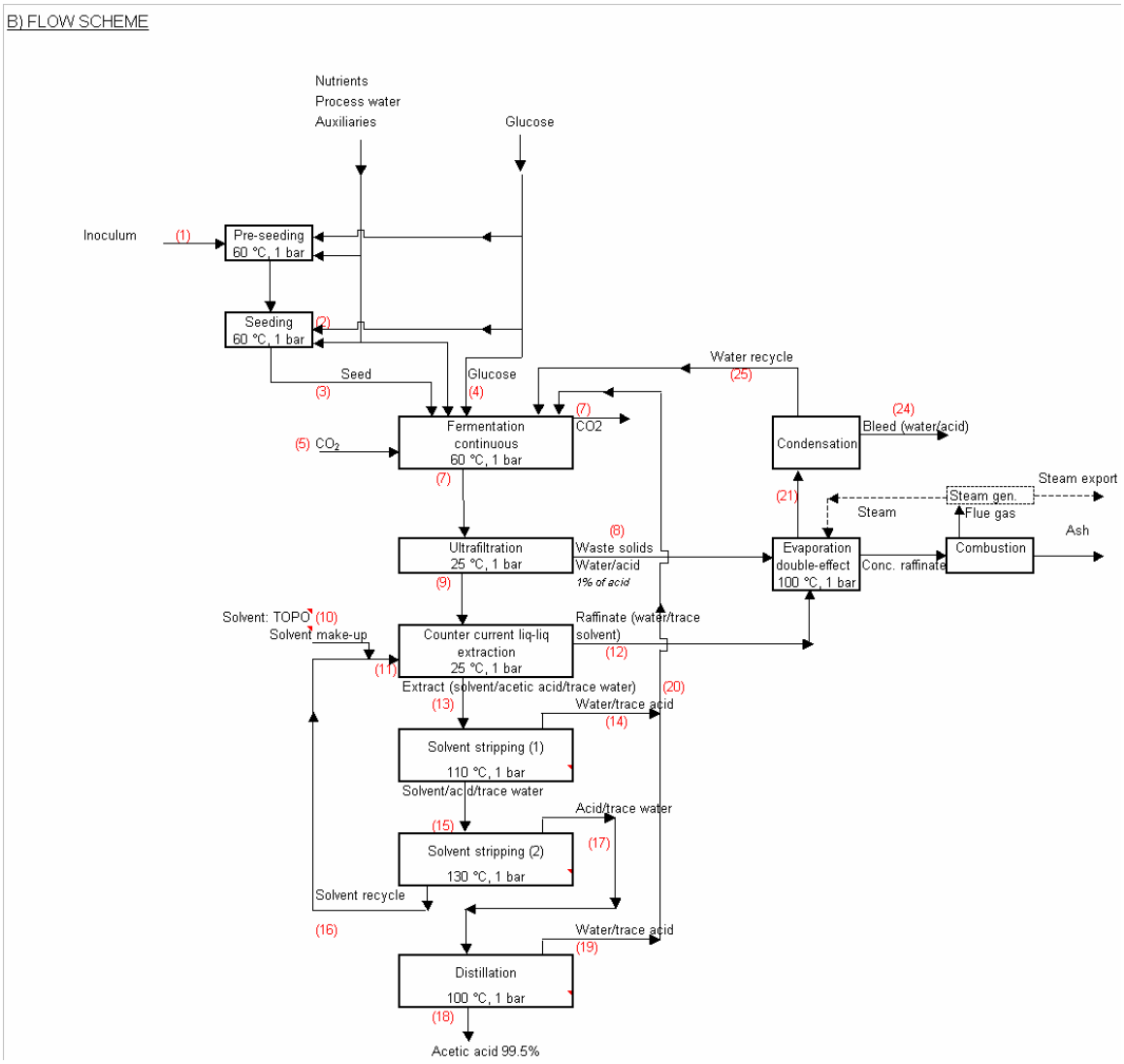
4.1 BioAcet-Anaer-GA-TexTOPO



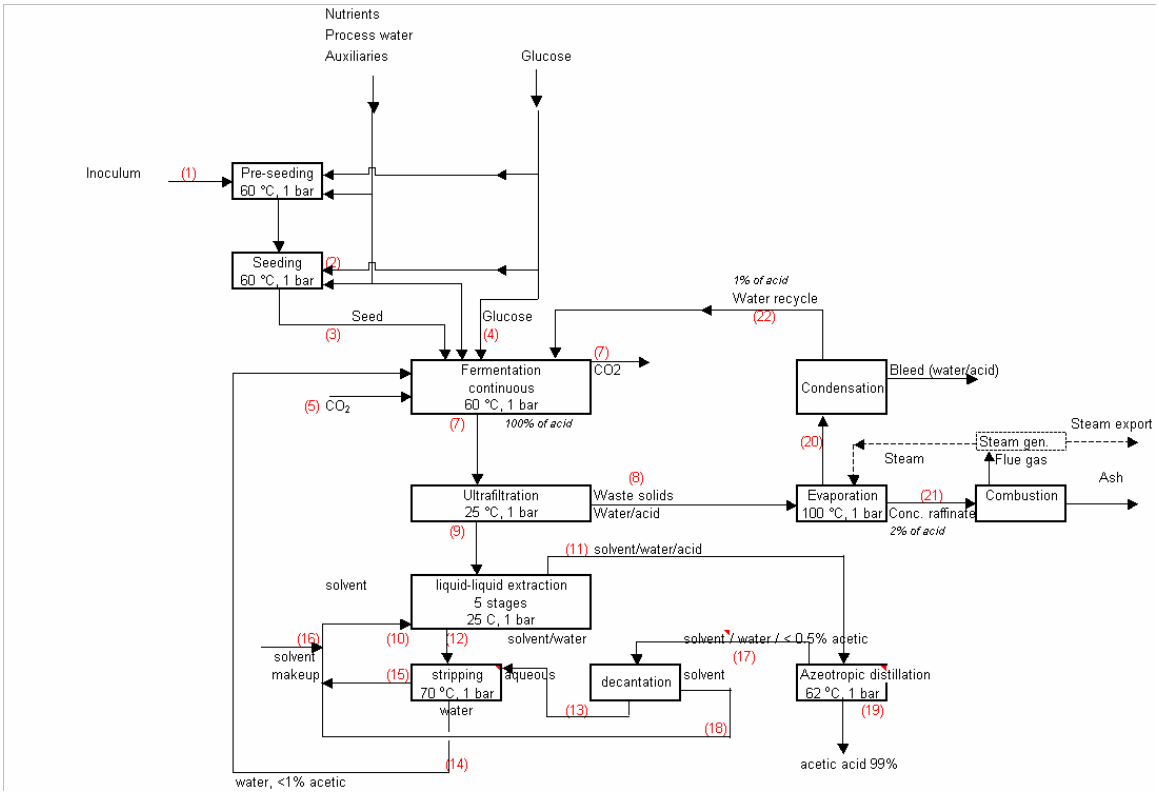
4.2 BioAcet-Anaer-GA-Ted



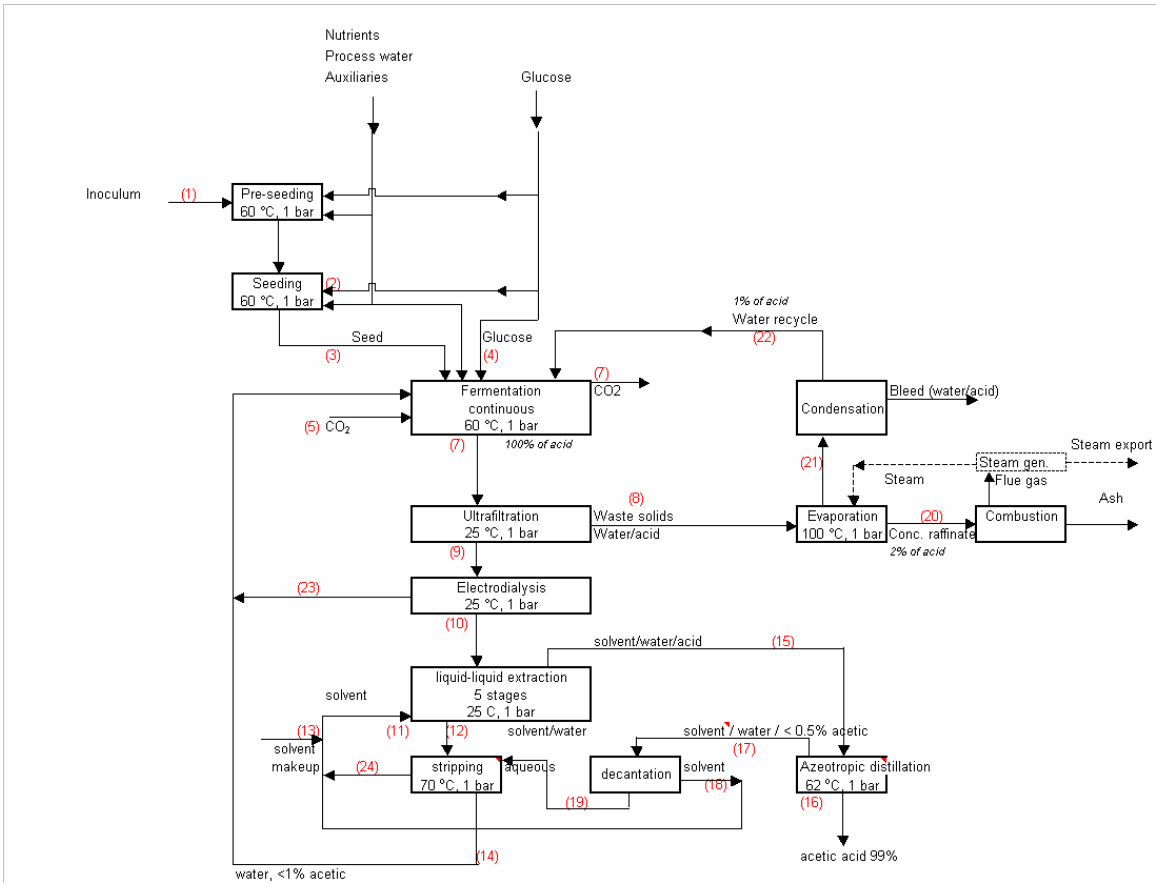
4.3 BioAcet-Anaer-GA-FexTOPO



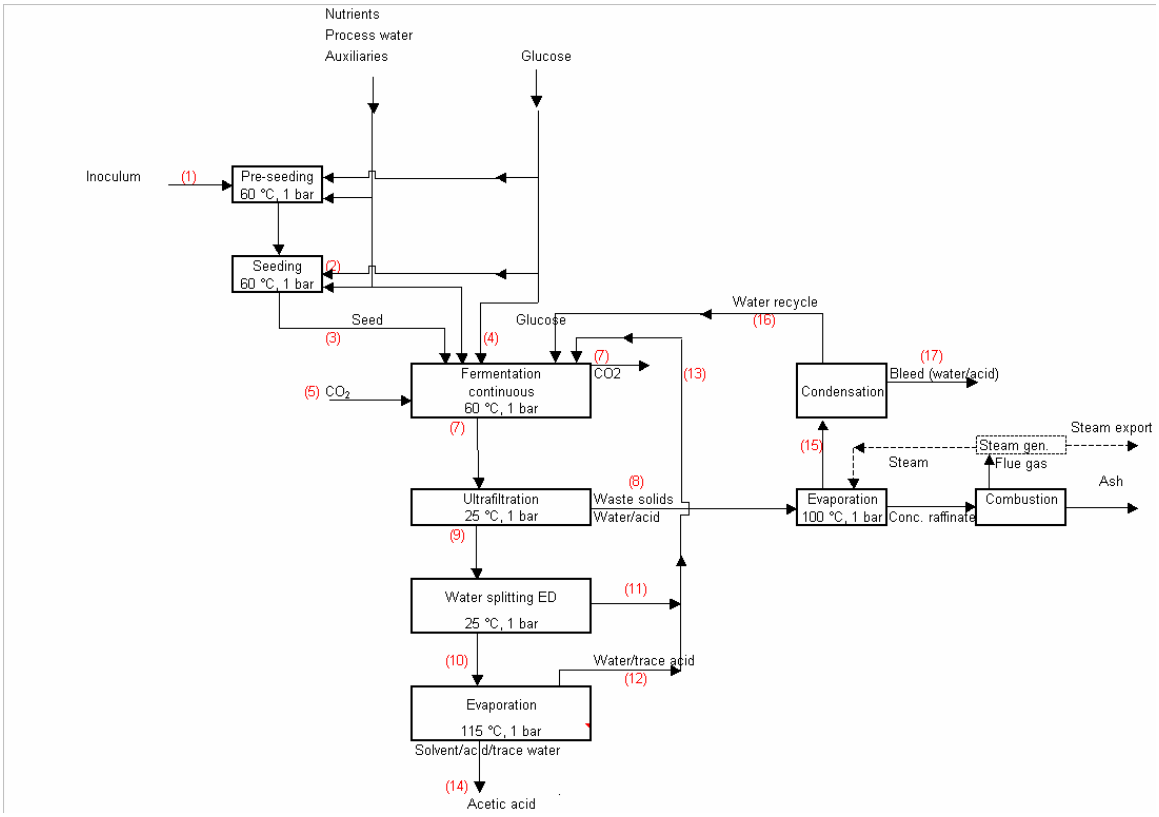
4.4 BioAcet-Anaer-GA-FexDIPE



4.5 BioAcet-Anaer-GA-FedexDIPE

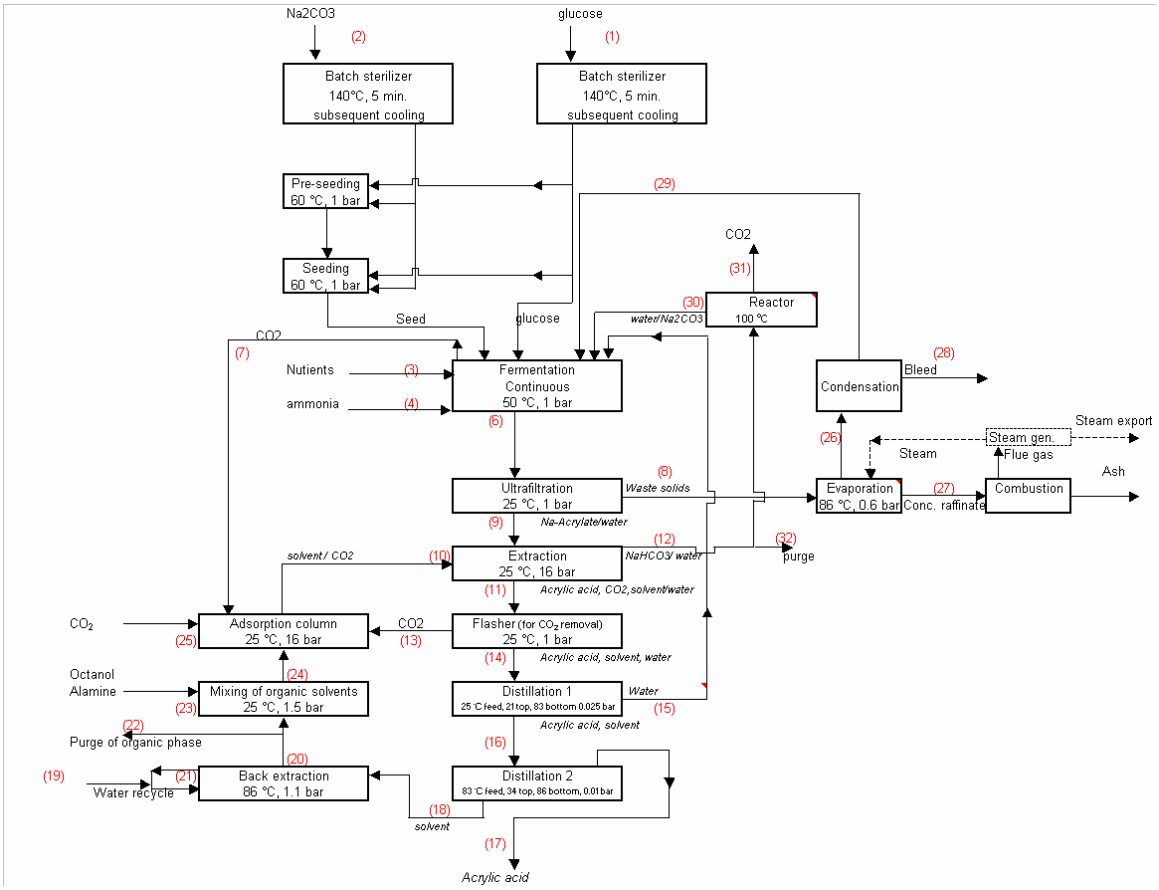


4.6 BioAcet-Anaer-GA-Fed



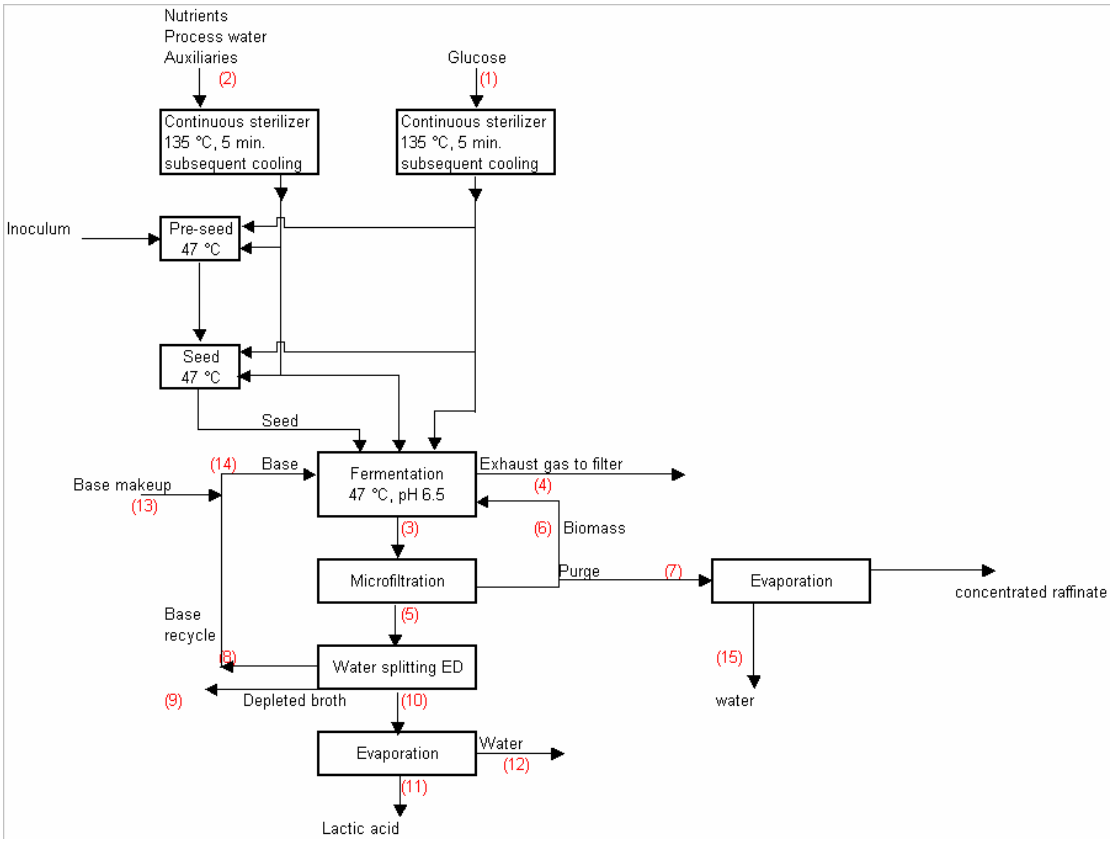
5. Acrylic acid

5.1 BioAcryl-Anaer-GA-Fex



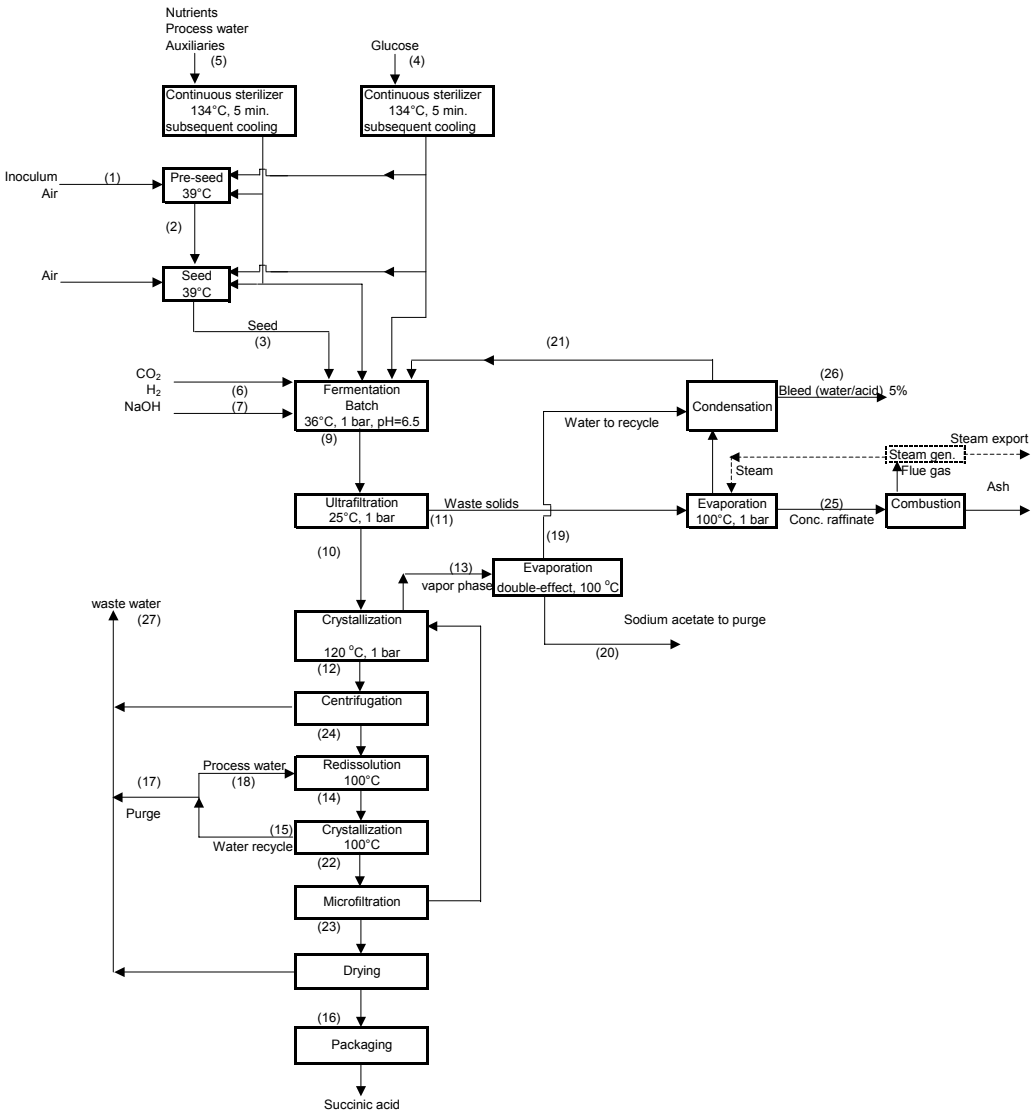
6. Lactic acid

6.1 BioLA-Anaer-GA-Fed

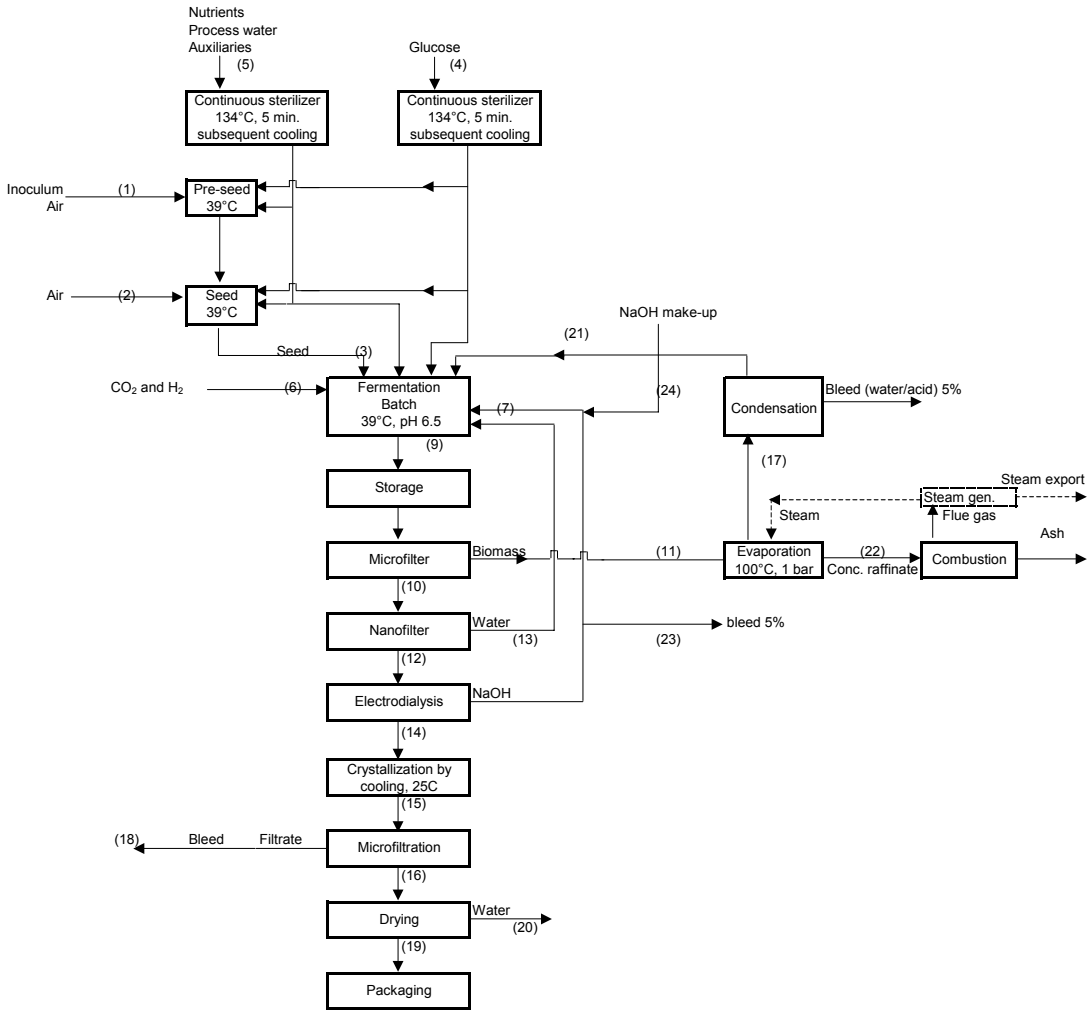


7. Succinic acid

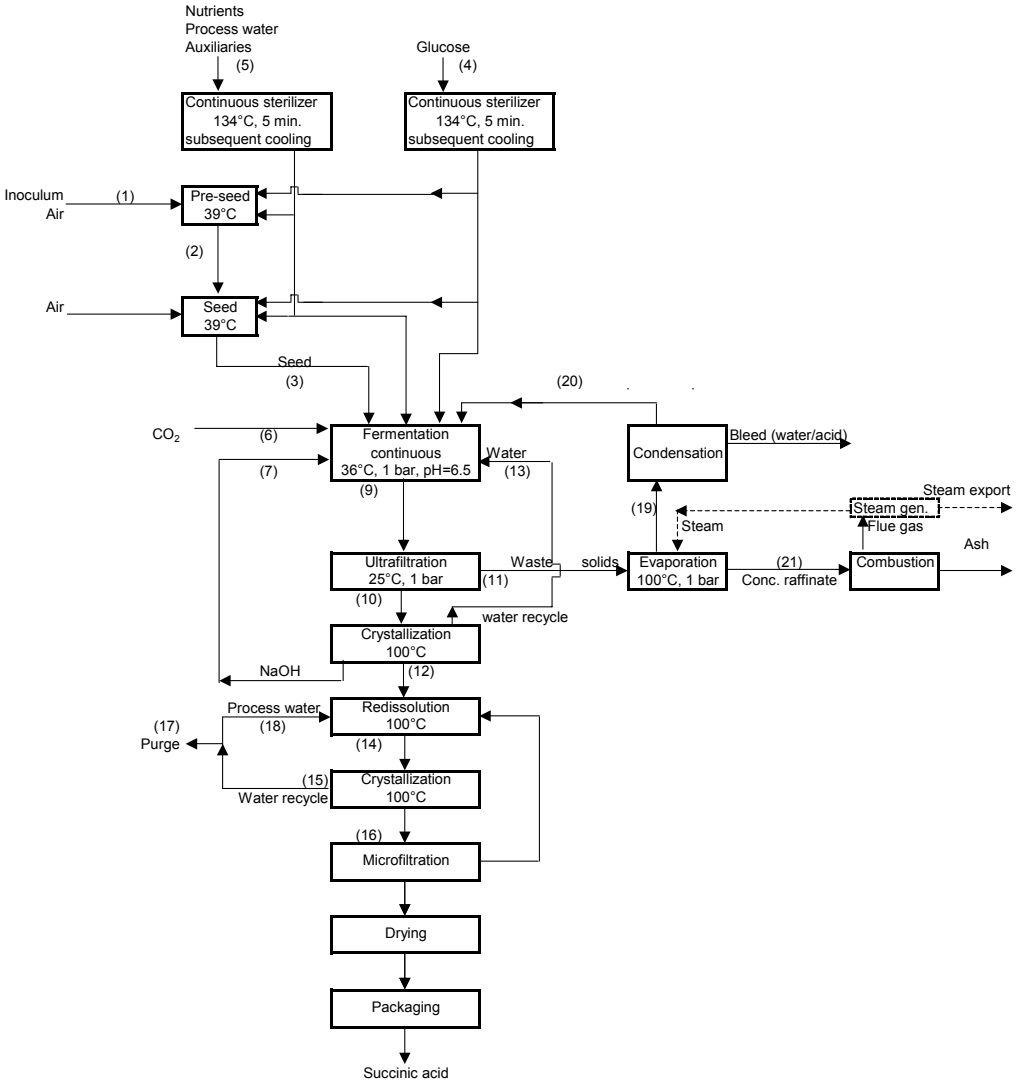
7.1 BioSA-Anaer-GA-Tc



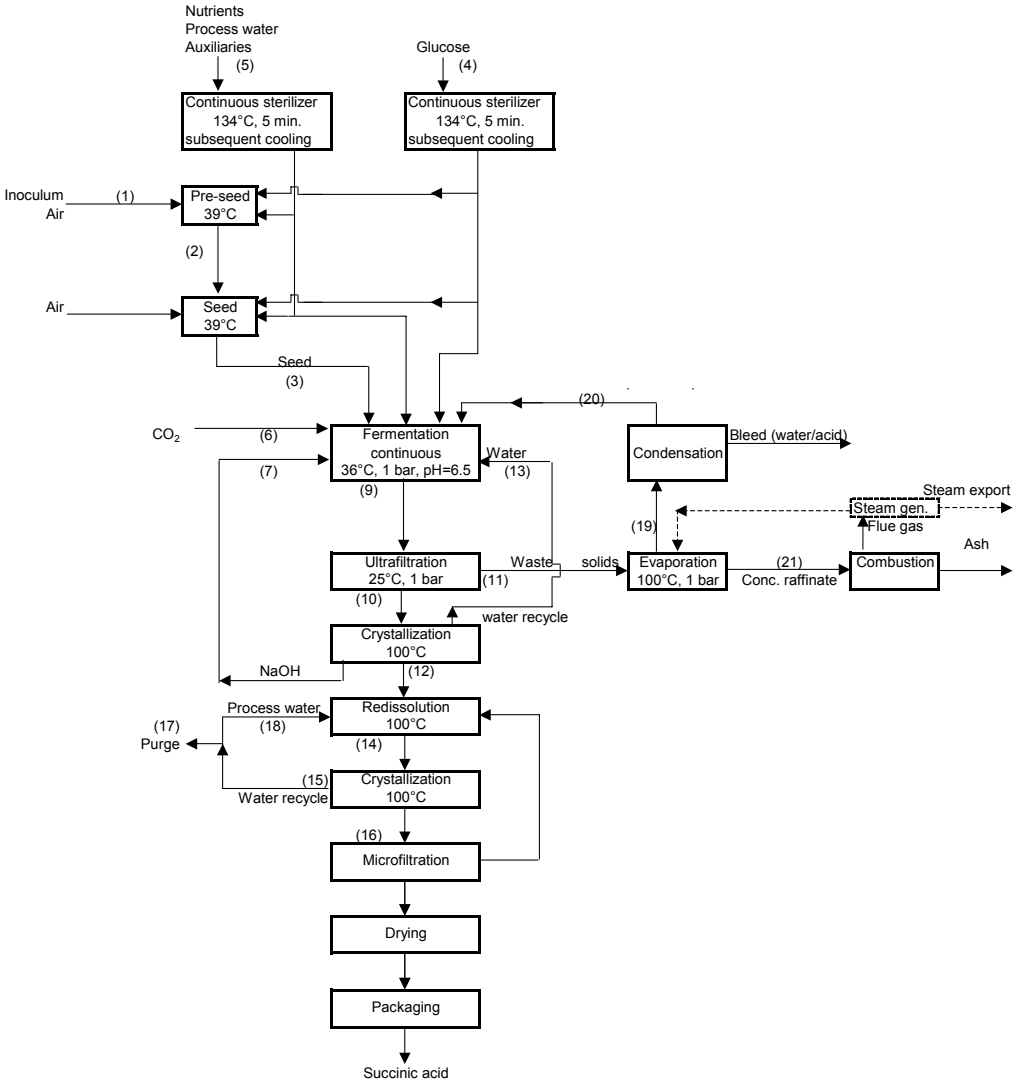
7.2 BioSA-Anaer-GA-Ted



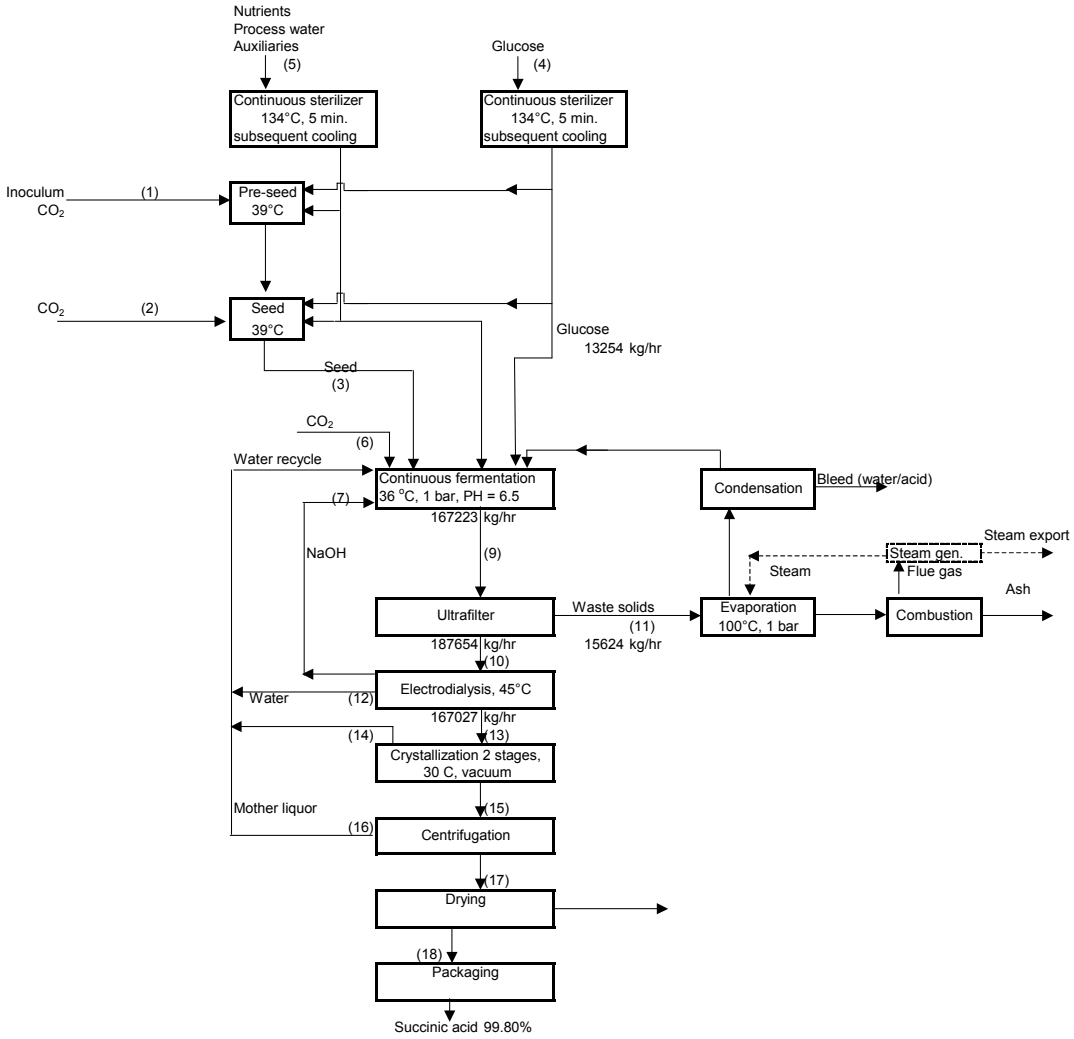
7.3 BioSA-Anaer-GA-Fcrx



7.4 BioSA-Anaer-GA-Fc

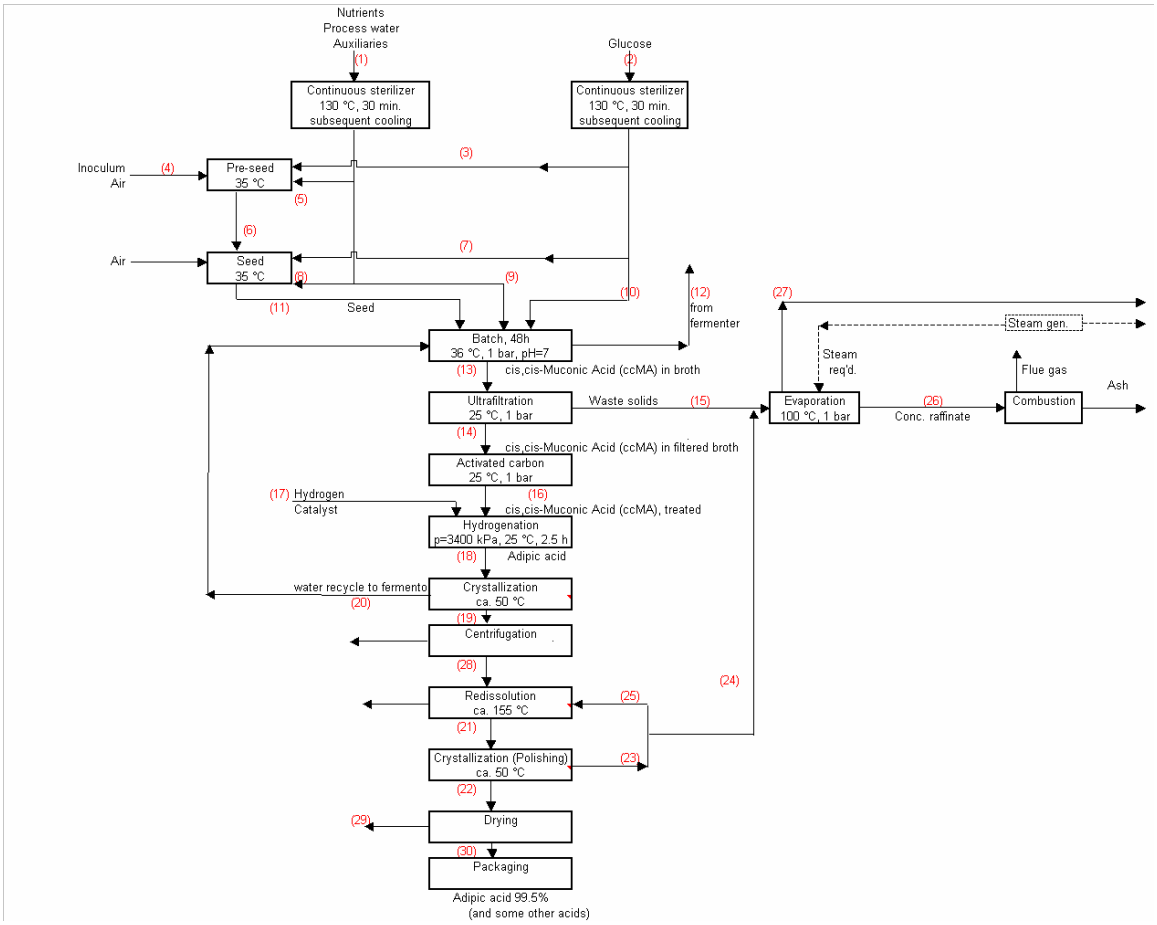


7.5 BioSA-Anaer-GA-Fed

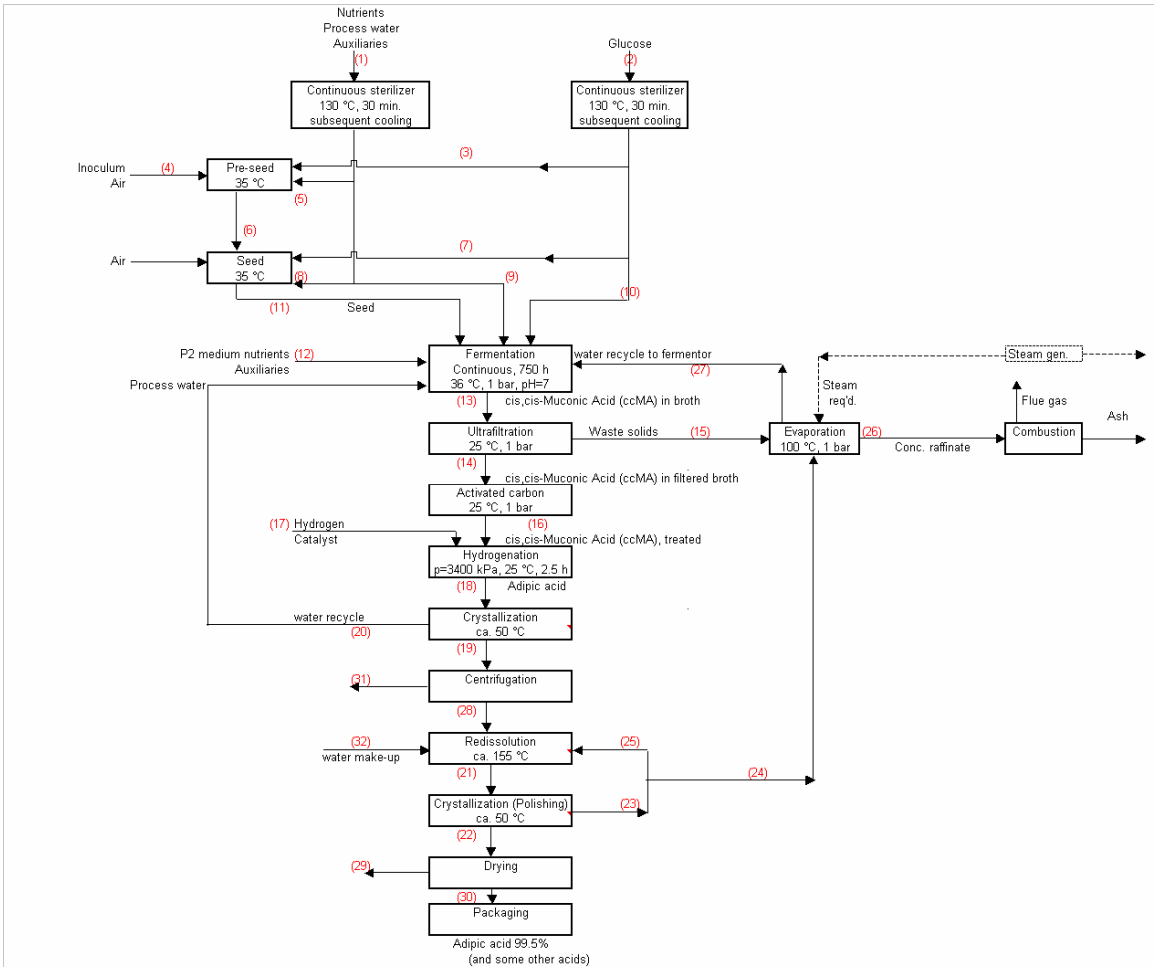


8. Adipic acid

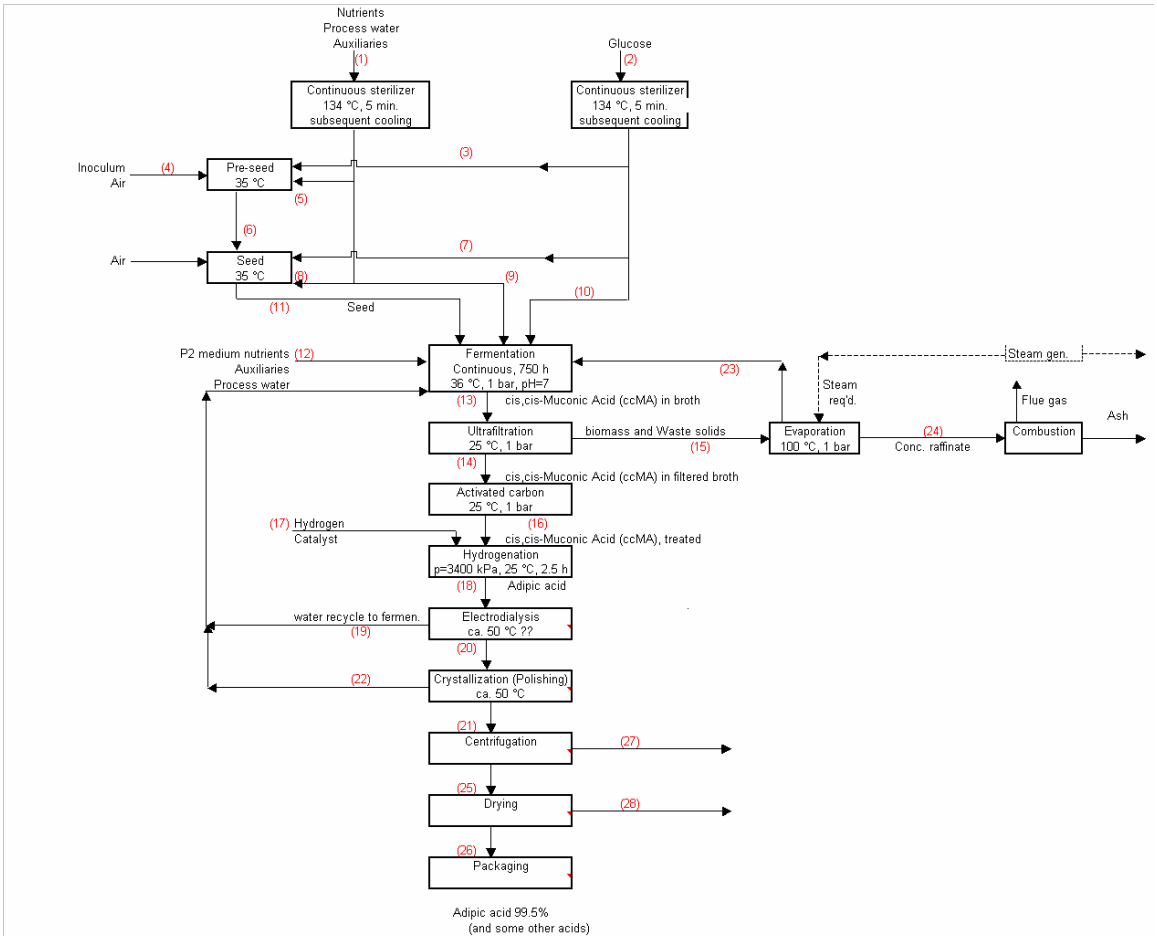
8.1 BioAdip-Aer-GA-Tc



8.2 BioAdip-Aer-GA-Fc

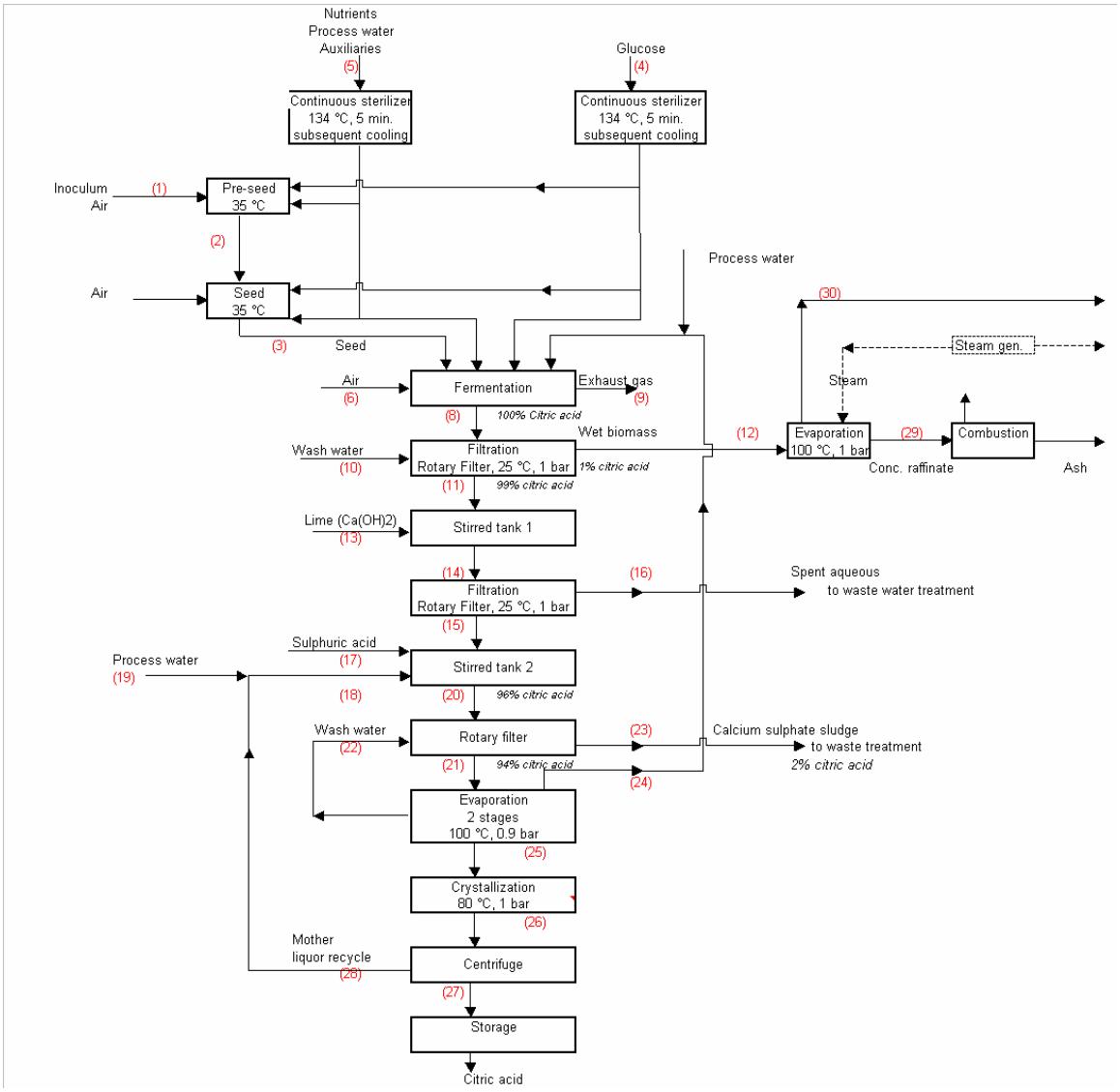


8.3 BioAdip-Aer-GA-Fed

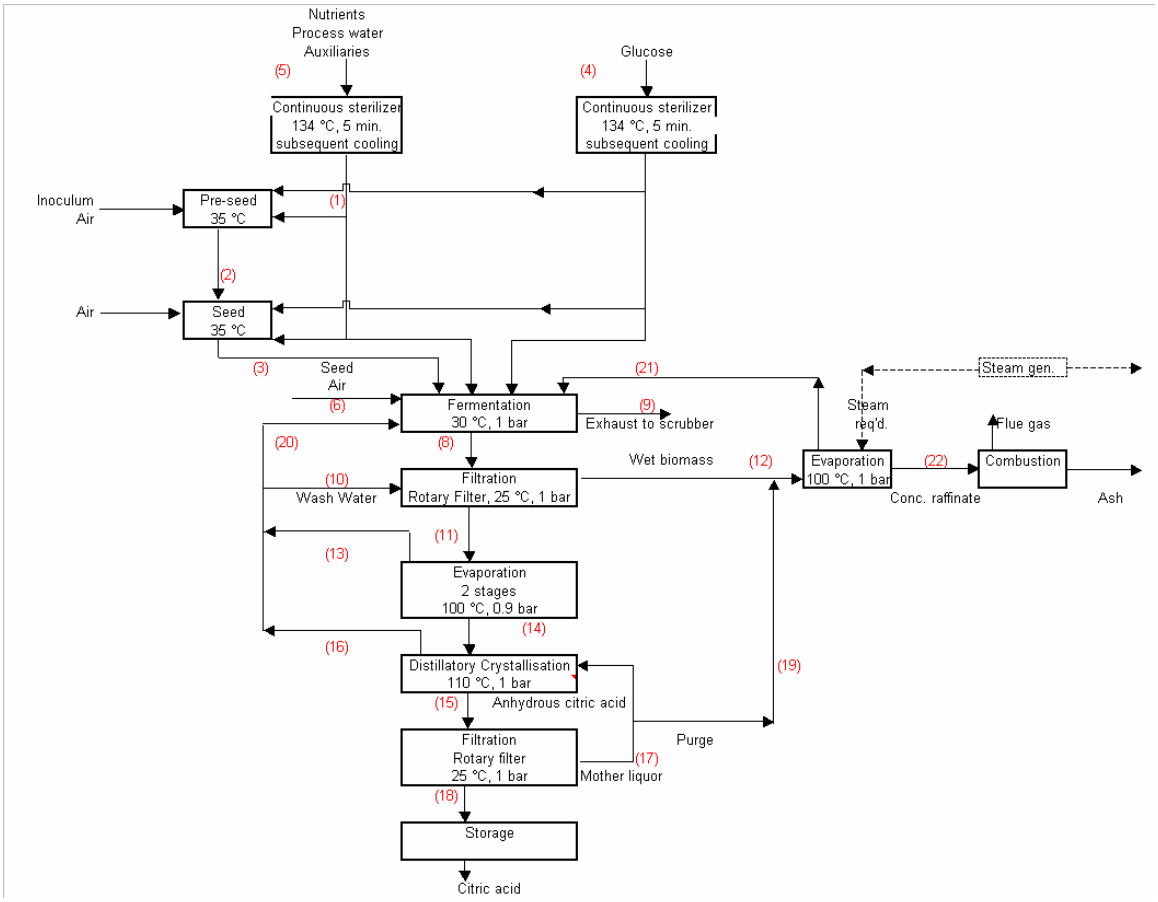


9. Citric acid

9.1 BioCit-Aer-GA-Tpc

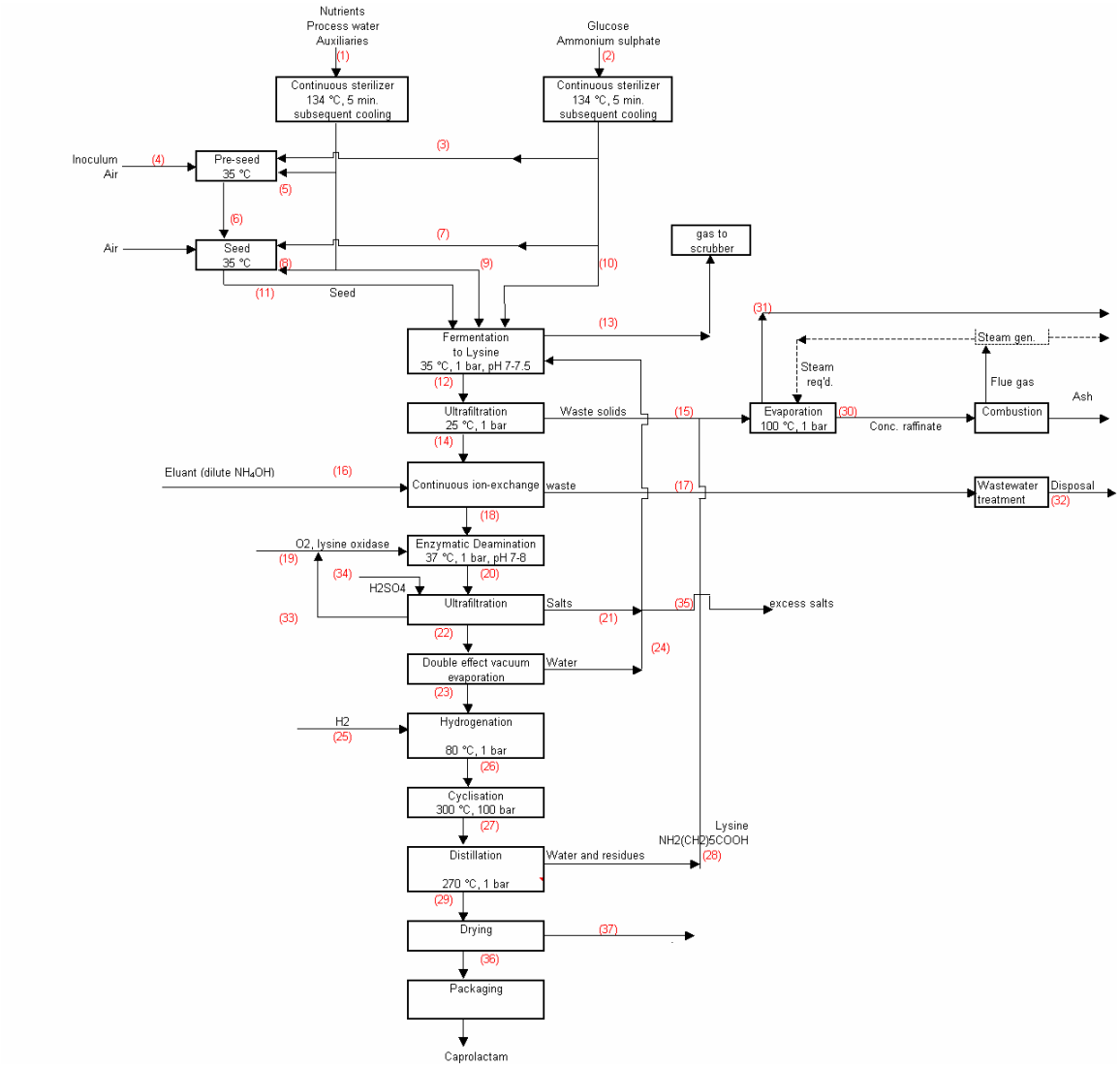


9.2 BioCit-Aer-GA-Fc



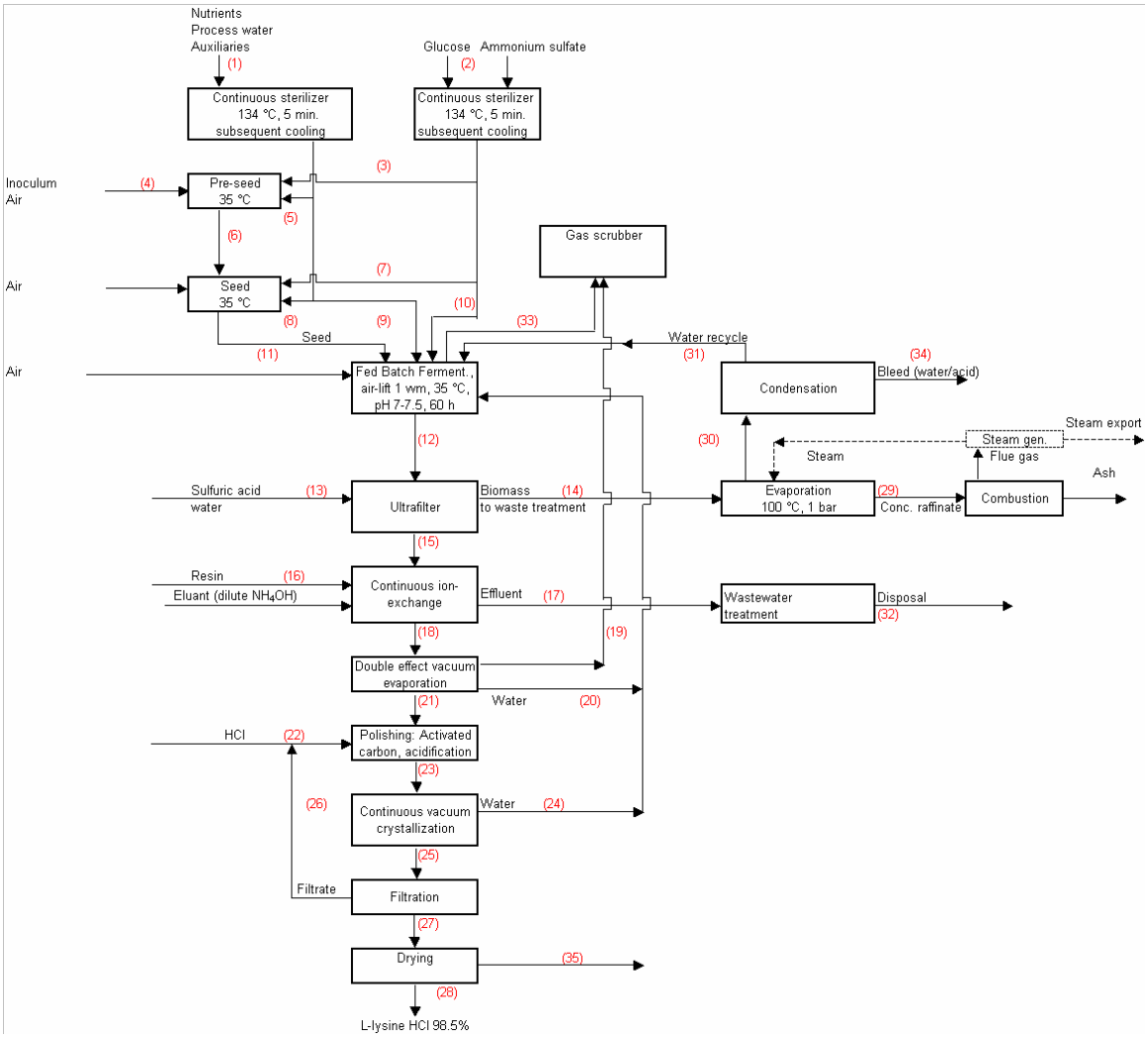
10. Caprolactam

10.1 BioCapro-Aer-GA-Fd

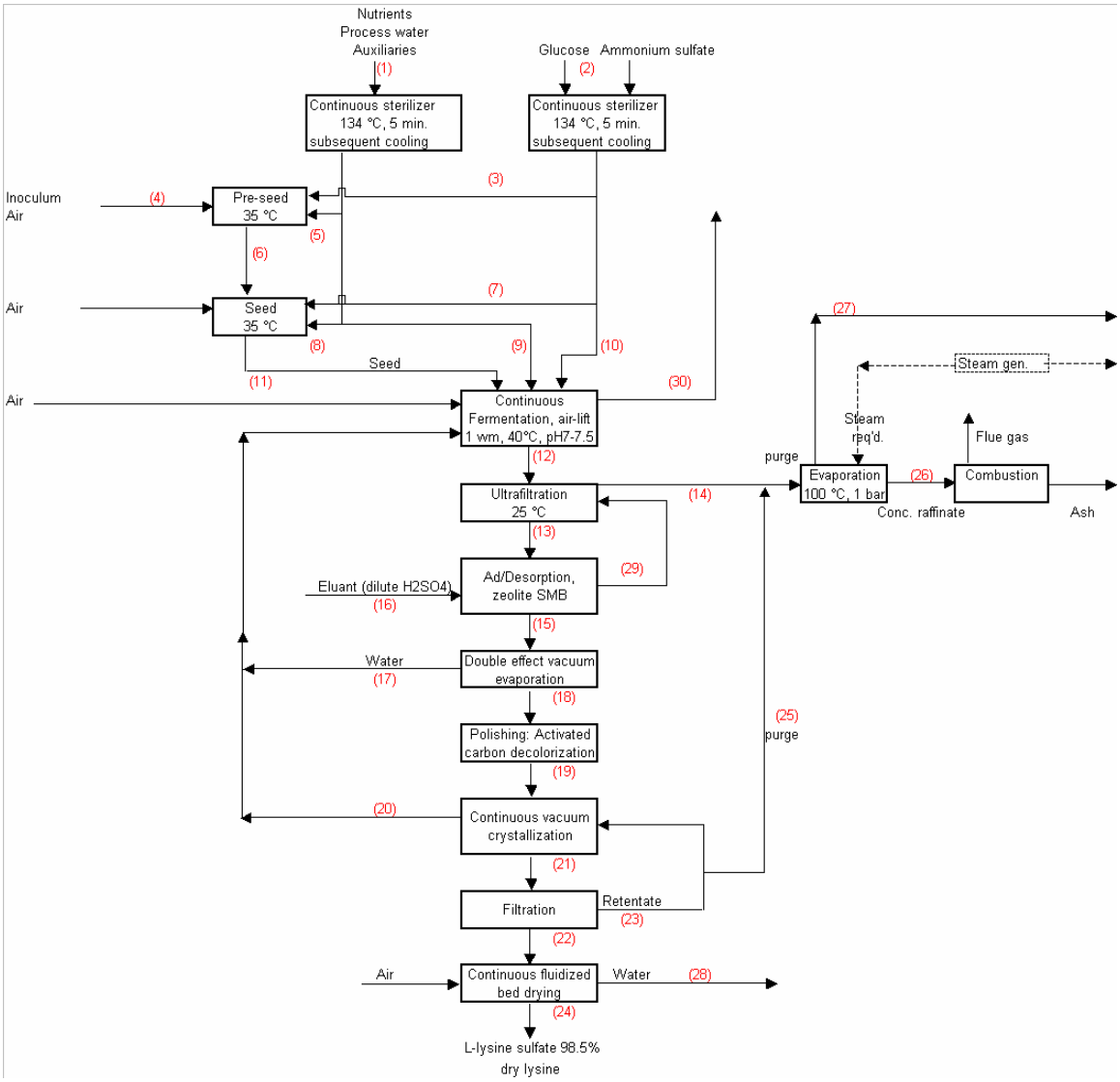


11. Lysine

11.1 BioLys-Aer-GA-Tix

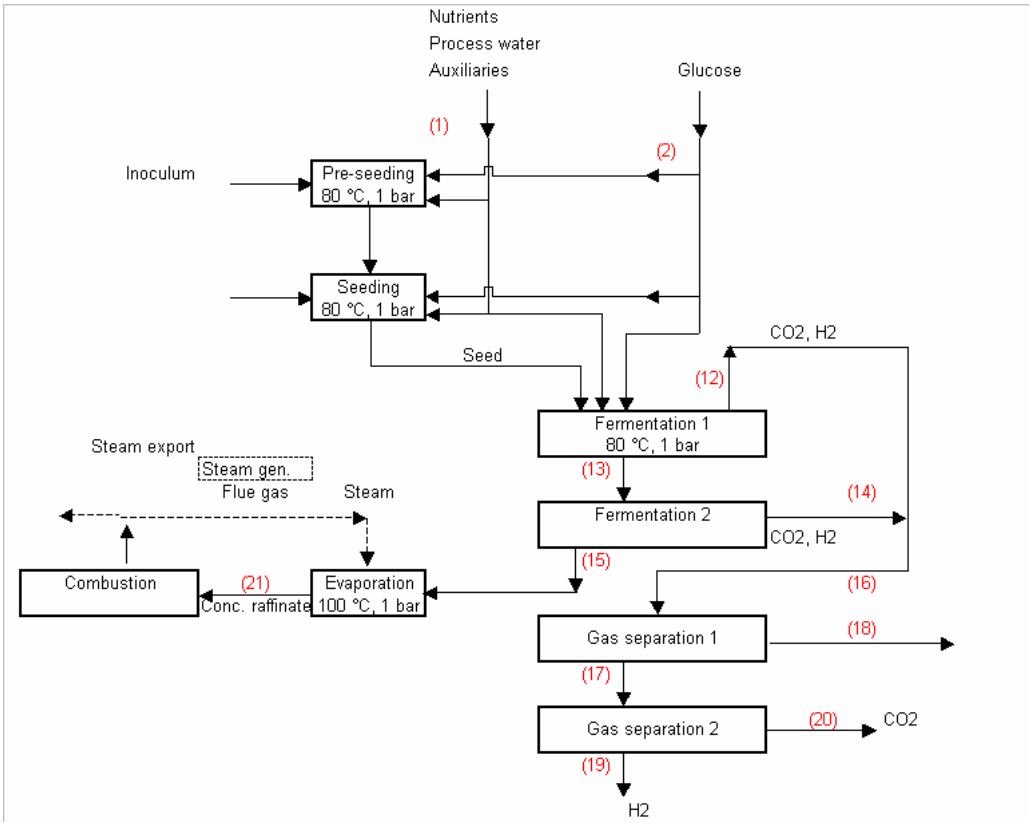


11.2 BioLys-Aer-GA-Fad



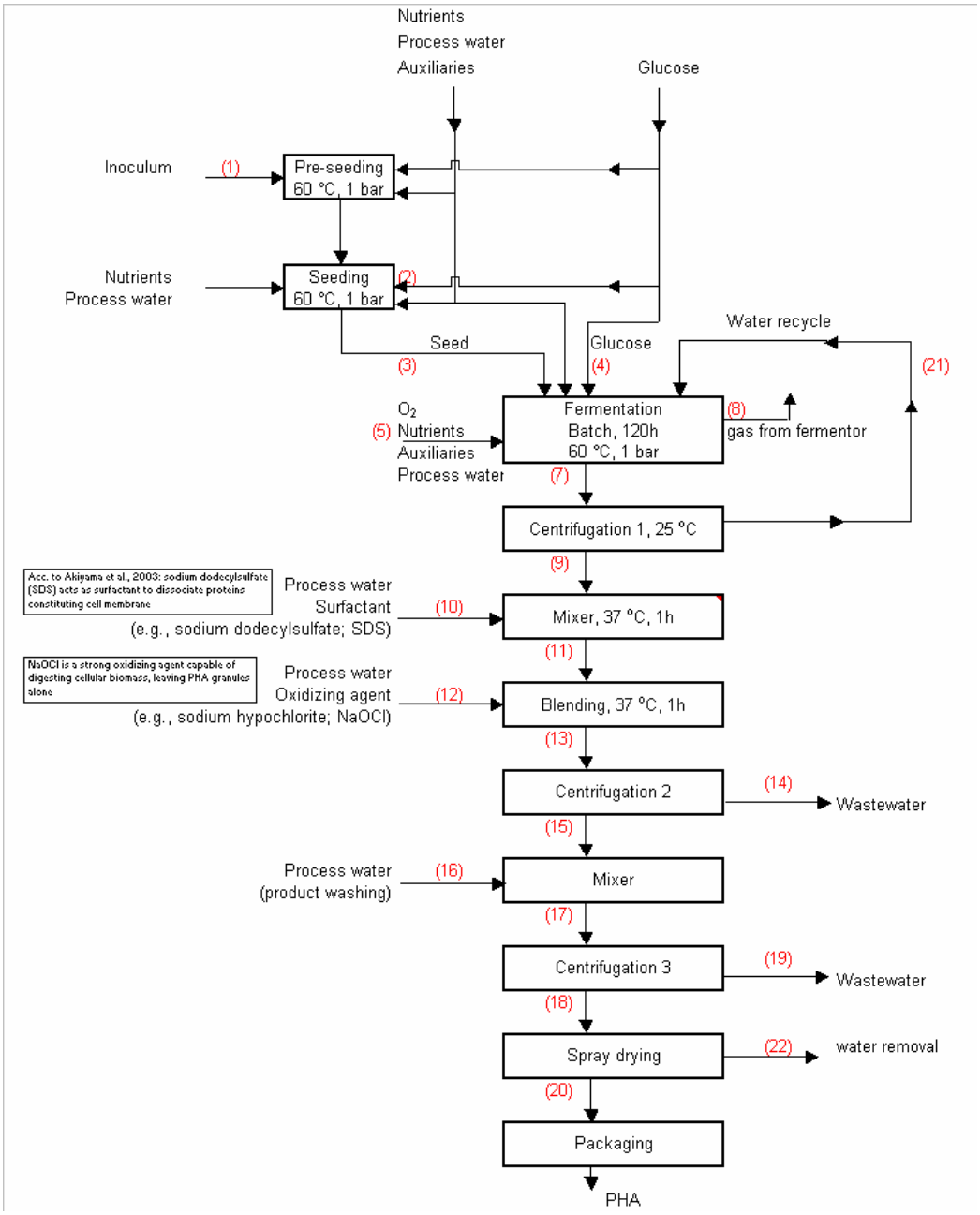
12. Hydrogen

12.1 BioH2-A&F-gs

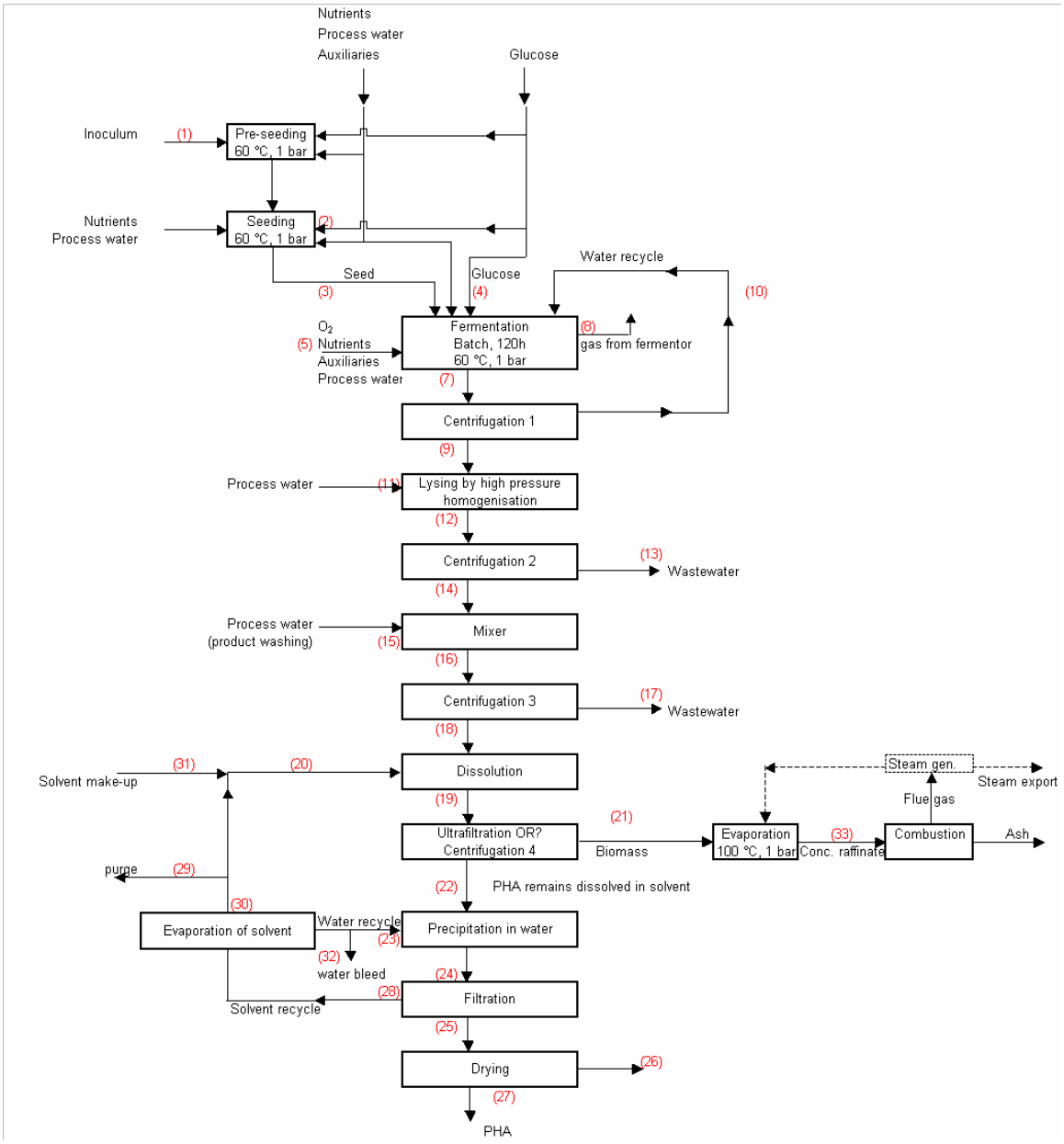


13. **PHA**

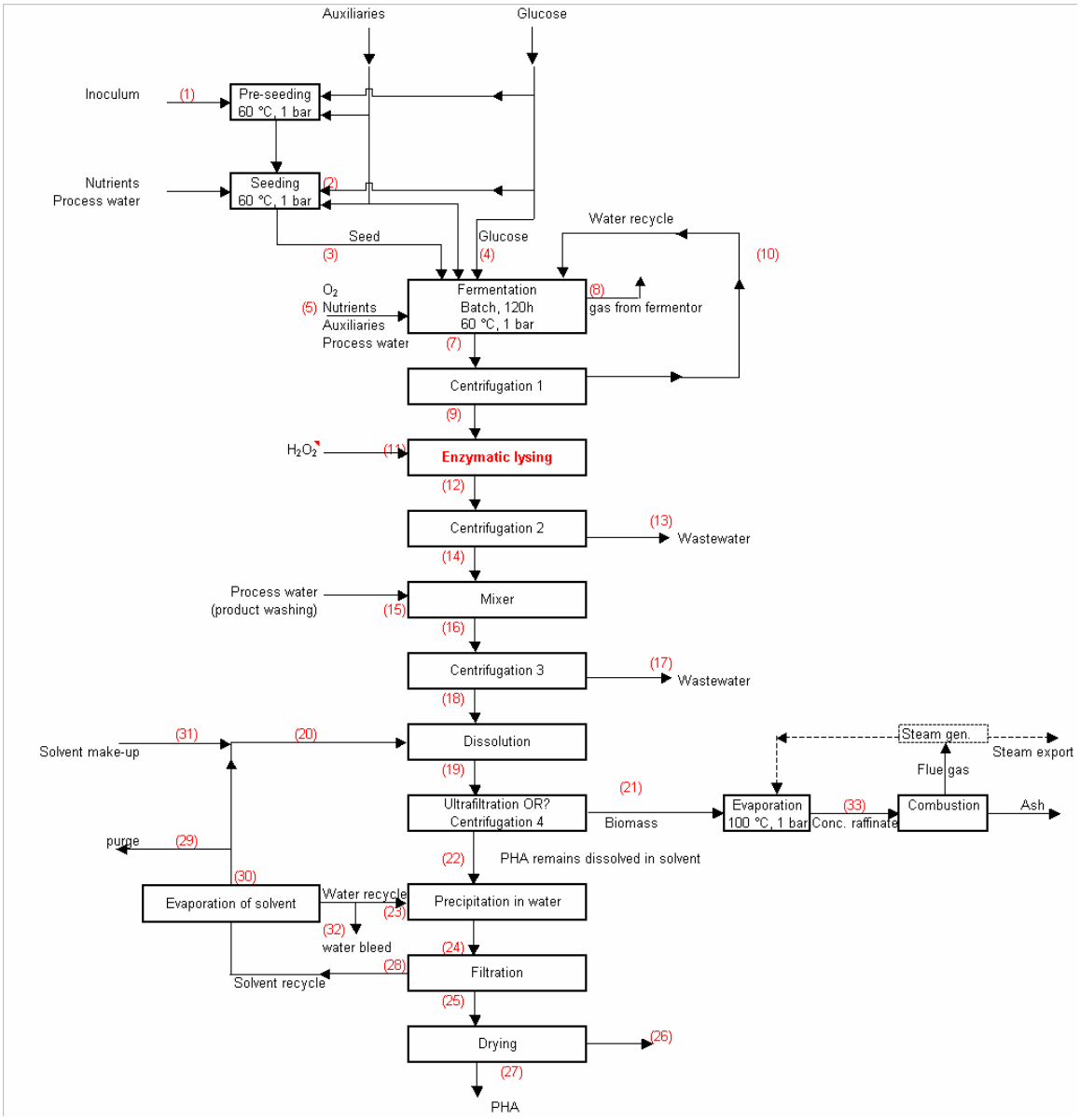
13.1 BioPHA-GA-Toa



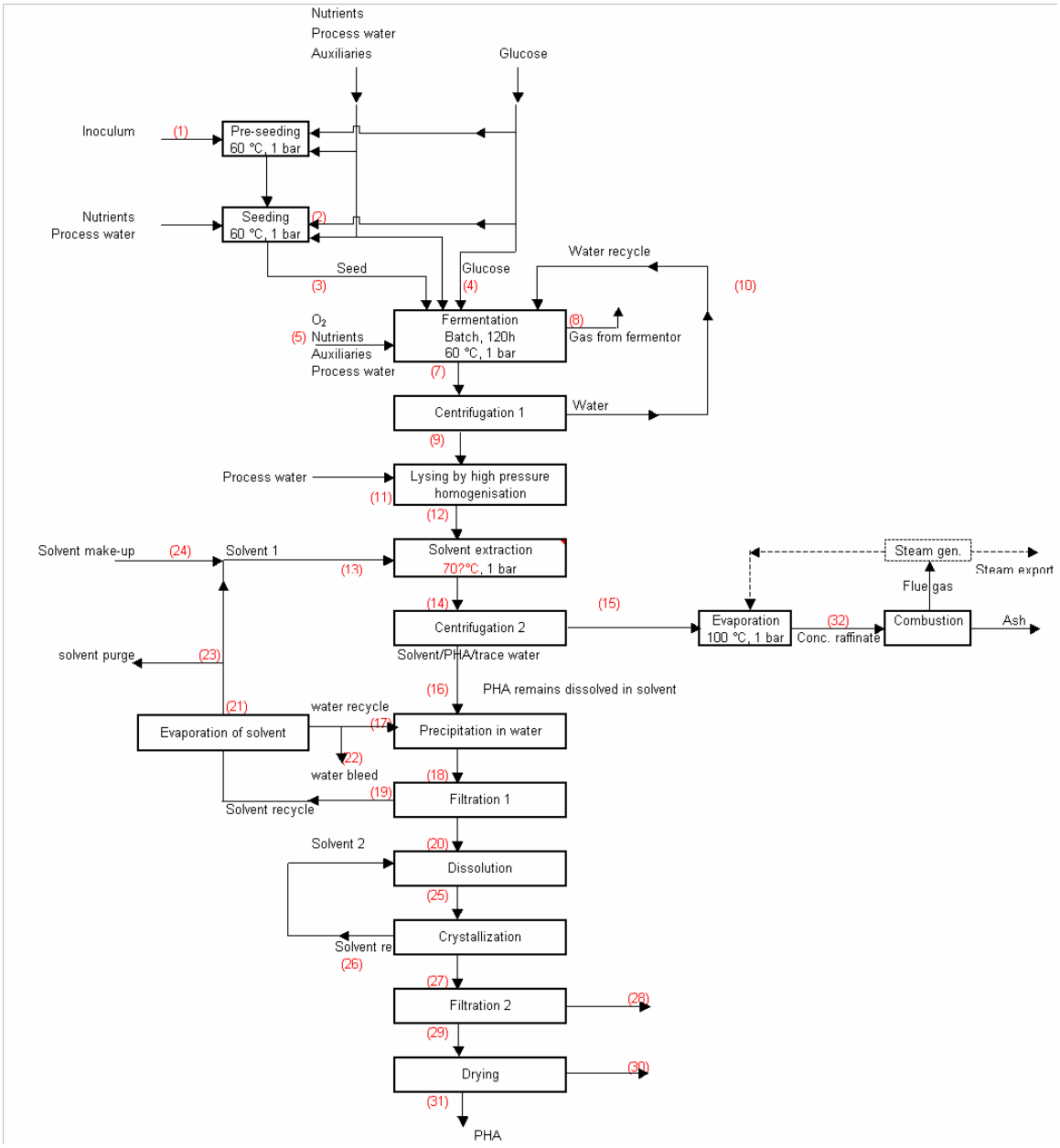
13.2 BioPHA-GA-Th



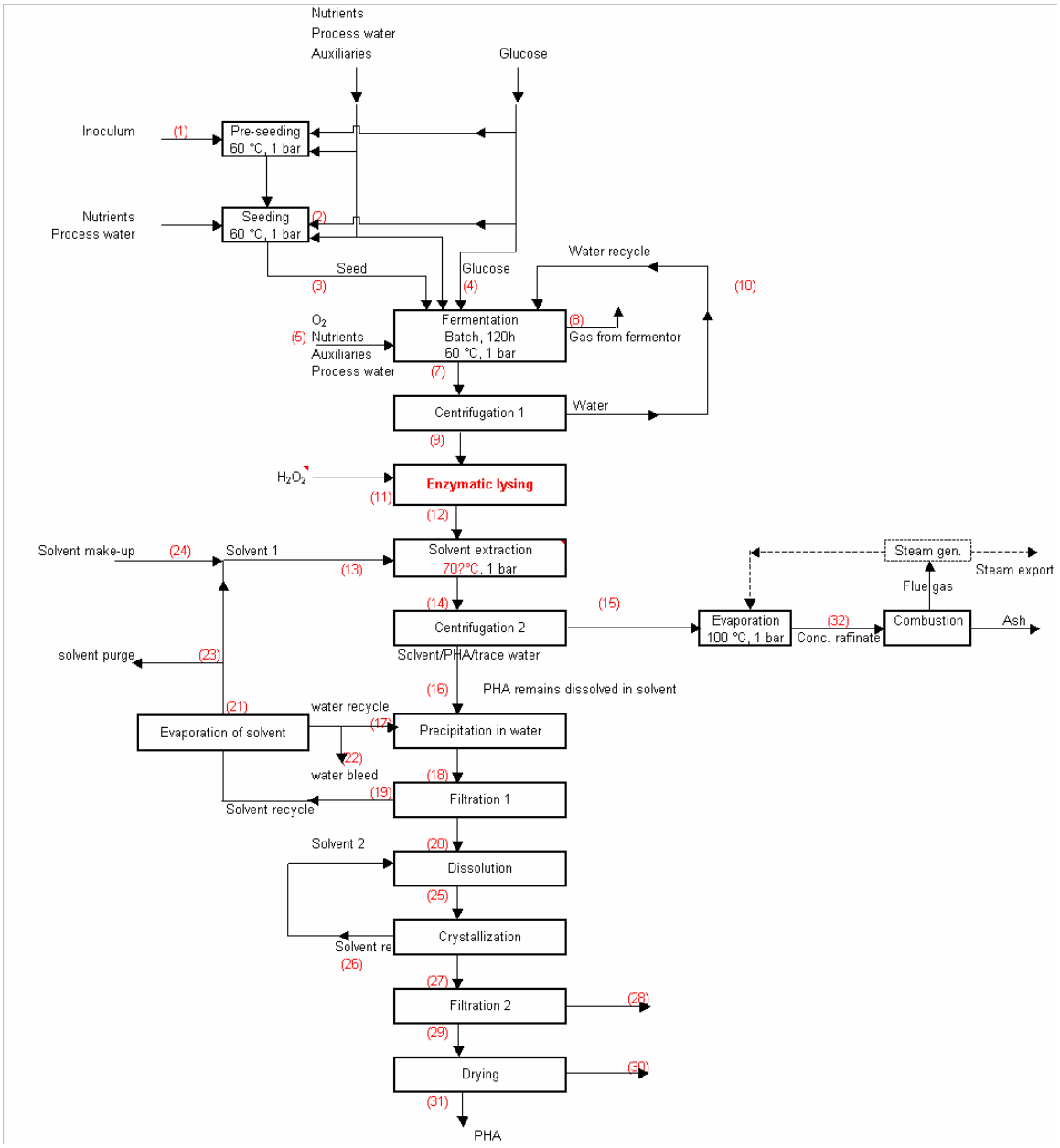
13.3 BioPHA-GA-Tey



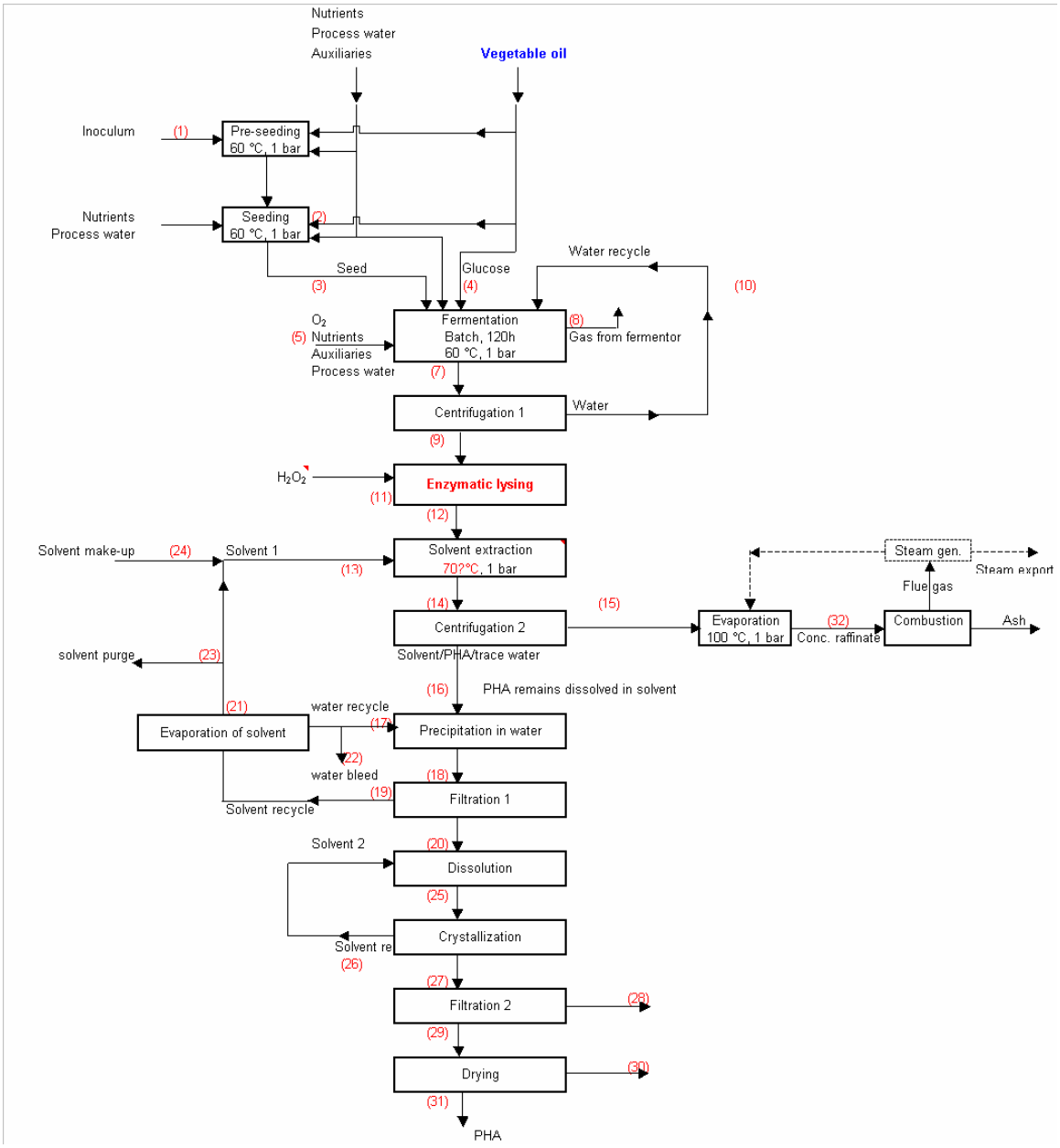
13.4 BioPHA-GA-Tex



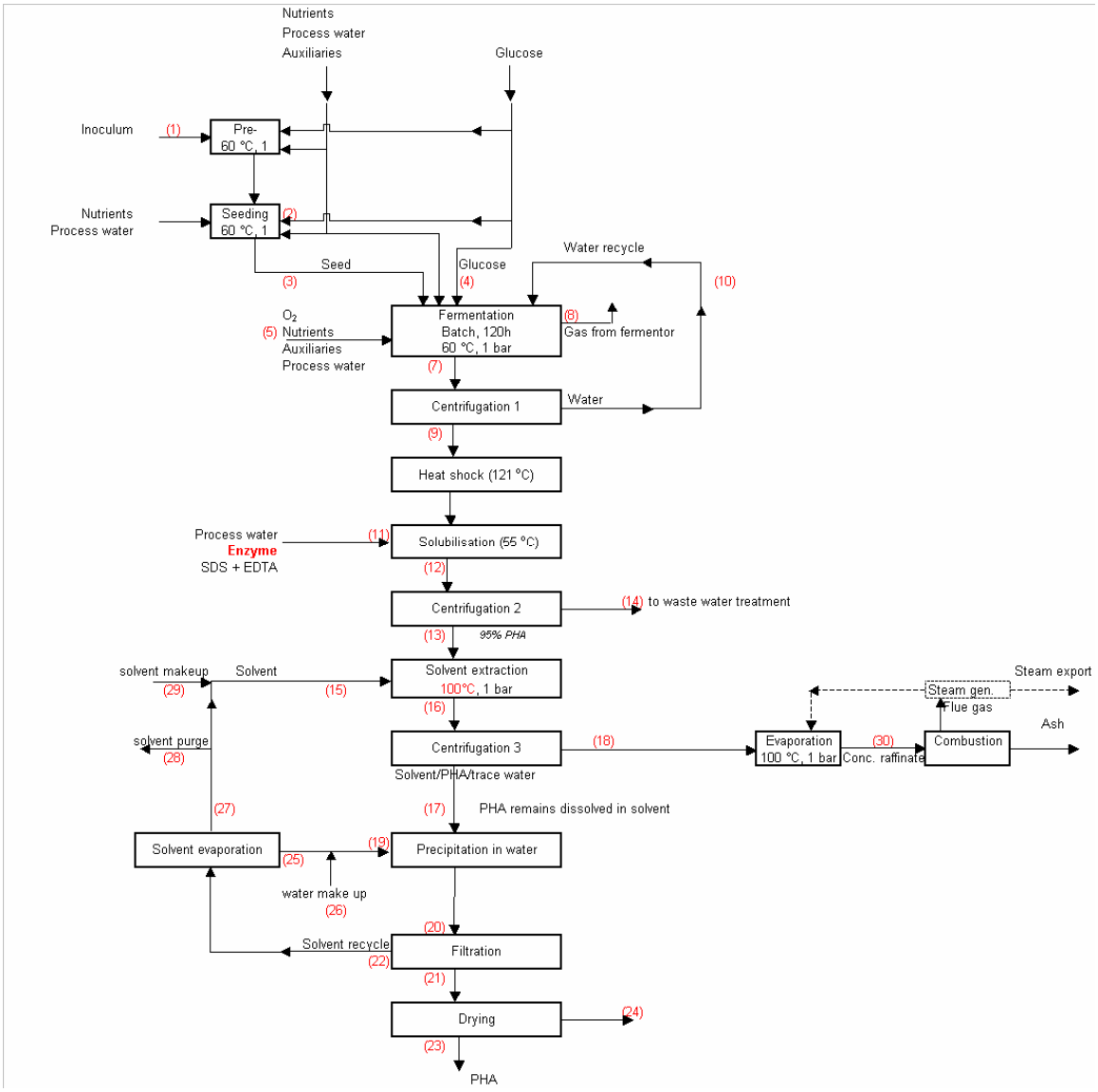
13.5 BioPHA-GA-Texey



13.6 BioPHA-GA-OilTexey



13.7 BioPHA-GA-Fey-1



Appendix 10: Results of techno-economic analyses in tabular form

Table of contents of Appendix 10:

(2 pages each for all tables listed below)

This appendix contains the results for non-renewable energy use (NREU), renewable energy use (REU) and greenhouse gas (GHG) emissions for all processes studied. A comparative overview of the non-renewable energy requirements (cradle-to-factory gate) across the three feedstocks (maize starch, lignocellulosics and sugar cane) can be found in Table 3-7 in the main text. Table 3-7 contains also the results for **land use**. The results of the **economic analyses** are given Table 3-9 in the main text.

Table A10-3a): Energy use for bio-based and equivalent petrochemical-based platform chemicals and products – Sugar from STARCH

			Non-renewable and renewable energy use on a cradle-to-factory gate basis			Non-renewable energy use on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	Non-renewable energy use	Renewable energy use	Total energy use	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Maize Starch	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)
Alcohols	Ethanol	BioEtOH-SRI-Td	27.1	38.0	65.1	27.1	13.4	18.7
		BioEtOH-SRI-Corn-Td	24.7	19.0	43.7	24.7	11.1	16.4
		BioEtOH-Anaer-GA-Tdcont	23.9	38.8	62.7	23.9	10.3	15.6
		BioEtOH-Anaer-GA-Fd	20.4	37.3	57.7	20.4	6.8	12.1
		BioEtOH-Anaer-GA-Fpv	18.2	37.3	55.5	18.2	4.6	9.9
		BioEtOH-SRI-Stover-Fd [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemEtOH-1 [2)]	63.9	0.0	63.9	63.9	50.2	55.6
		PchemEtOH-2 [2)]	54.2	0.0	54.3	54.2	40.6	45.9
	PDO	BioPDO-Anaer-SRI-Tdcont	54.6	37.1	91.7	54.6	43.0	47.5
		BioPDO-Aer-SRI-Tdcont	46.4	29.6	76.0	46.4	34.8	39.3
		BioPDO-Aer-DP-Tu	40.9	39.3	80.3	40.9	29.4	33.9
		BioPDO-Aer-GA-Tevbat	53.1	42.1	95.2	53.1	41.5	46.0
		BioPDO-Aer-GA-Tevcont	37.6	42.1	79.7	37.6	26.0	30.5
		BioPDO-Aer-GA-FpvH2O	43.2	33.1	76.3	43.2	31.7	36.2
		BioPDO-Aer-GA-FpvPDO	19.8	33.1	52.9	19.8	8.2	12.7
		BioPDO-Anaer-Glyc-SRI-Tdcont [3)]	62.8	42.7	105.5	62.8	51.2	55.7
		BioPDO-Anaer-Glyc-VDI-Tdbat [3)]	63.5	33.4	96.8	63.5	51.9	56.4
		PchemPDO-Propyl-DP	91.5	0.0	91.5	91.5	79.9	84.4
		PchemPDO-EO-SRI	69.1	0.0	69.1	69.1	57.6	62.1
		PchemPDO-Acro-SRI	101.2	0.0	101.3	101.2	89.7	94.2
	ABE	BioABE-Anaer-GA-Tdcont	63.9	51.9	115.8	63.9	47.4	53.8
		BioABE-Anaer-GA-Tgscont	57.2	51.9	109.1	57.2	40.7	47.1
		BioABE-Anaer-GA-Fdm	29.0	43.6	72.6	29.0	12.5	18.9
		BioABE-Anaer-GA-Fmd	6.6	43.6	50.2	6.6	-10.0	-3.5
		BioABE-Anaer-GA-Fpv	7.9	43.6	51.5	7.9	-8.7	-2.2
		BioABE-Anaer-GA-Fgs	18.1	43.6	61.7	18.1	1.6	8.0
		PchemButanol	69.3	0.0	69.3	69.3	52.7	59.2
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	144.9	35.9	180.7	144.9	137.7	140.5
		BioAcet-Anaer-GA-Ted	108.9	35.5	144.4	108.9	101.8	104.6
		BioAcet-Anaer-GA-FexTOPO	57.4	19.7	77.1	57.4	50.3	53.1
		BioAcet-Anaer-GA-FexDIPE	64.9	20.0	84.9	64.9	57.7	60.5
		BioAcet-Anaer-GA-FedexDIPE	38.9	19.8	58.7	38.9	31.8	34.5
		BioAcet-Anaer-GA-Fed	43.7	19.7	63.4	43.7	36.5	39.3
		PchemAceticAcid	55.5	0.0	55.5	55.5	48.6	51.3
	Acrylic acid	BioAcryl-Anaer-GA-Fex	30.8	24.1	54.9	30.8	22.2	25.6
		PchemAcrylicAcid	47.1	0.0	47.1	47.1	38.5	41.9
	Lactic acid	BioLA-SRI-TpH6cont	37.5	20.6	58.0	37.5	30.3	33.1
		BioLA-SRI-FlowpH	36.8	29.3	66.1	36.8	29.6	32.4
		BioLA-NW-Tu	31.2	20.7	51.9	31.2	24.0	26.8
		BioLA-Sh-Fex	28.5	29.3	57.8	28.5	21.3	24.1
		BioLA-Sh-Fed	30.9	29.3	60.2	30.9	23.8	26.5
		BioLA-Anaer-GA-Fed	22.6	19.0	41.6	22.6	15.5	18.2
		BioLA-NW-Fu	19.6	19.3	38.9	19.6	12.4	15.2
	Succinic acid	BioSA-Anaer-GA-Tc	66.5	36.1	102.6	66.5	60.4	62.8
		BioSA-Anaer-GA-Ted	27.0	34.7	61.7	27.0	20.8	23.2
		BioSA-Aer-SRI-Fed	45.6	21.2	66.7	45.6	39.4	41.8
		BioSA-Anaer-GA-Fcrx	32.4	21.9	54.3	32.4	26.3	28.7
		BioSA-Anaer-GA-Fc	46.8	20.1	66.9	46.8	40.6	43.0
		BioSA-Anaer-GA-Fed	28.0	20.8	48.7	28.0	21.8	24.2
		PchemMaleicAnhydride	67.7	1.2	69.0	67.7	61.9	64.2
		PchemSA-MalAnhydr	96.3	1.4	97.7	96.3	90.1	92.5
	Adipic acid	BioAdip-Aer-GA-Tc	195.4	100.1	295.6	195.4	186.6	190.0
		BioAdip-Aer-GA-Fc	59.6	36.7	96.3	59.6	50.7	54.2
		BioAdip-Aer-GA-Fed	44.3	37.5	81.8	44.3	35.4	38.9
		PchemAdipicAcid	85.5	0.0	85.5	85.5	76.6	80.1
	Citric acid	BioCit-Aer-SRI-Tevc [4)]	73.7	0.6	74.3	73.7	68.9	70.8
		BioCit-Aer-SRI-Tix	74.9	45.0	119.9	74.9	70.1	72.0
		BioCit-Aer-GA-Tpc	97.0	62.1	159.1	97.0	92.2	94.1
		BioCit-Aer-GA-Fc	22.1	18.6	40.6	22.1	17.3	19.1

[1)] The original process data used cover all steps starting with the intake of corn stover (for BioEtOH-SRI-Stover-Fd). The results are therefore given in the table for lignocellulosic inputs.

[2)] Dataset PchemEtOH-1 is based on SRI data while dataset PchemEtOH-2 originates from the project C-STREAMS (Patel et al, 1999).

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[4)] The original process data used refer to the use of cane molasses. For this reason results are only presented for sugar cane as feedstock type and *not* for maize starch and lignocellulosics.

			Non-renewable and renewable energy use on a cradle-to-factory gate basis			Non-renewable energy use on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	Non-renewable energy use	Renewable energy use	Total energy use	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Maize Starch	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	43.3	44.8	88.1	43.3	28.7	34.4
		PchemCapro	117.1	0.0	117.1	117.1	102.4	108.1
	Lysine	BioLys-Aer-SRI-Tix	189.1	50.6	239.7	189.1	176.2	181.3
		BioLys-Aer-SRI-Tsp	65.9	55.7	121.6	65.9	53.0	58.0
		BioLys-Aer-GA-Tix	168.7	79.7	248.4	168.7	155.8	160.8
		BioLys-Aer-GA-Fad	131.1	55.1	186.2	131.1	118.2	123.2
H_2	Hydrogen	BioH2-A&F-gs [1)]	14.4	184.2	198.6			
		PchemH2	180.0	0.0	180.0			
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	64.7	64.6	129.3	64.7	47.9	54.4
		BioPHAmcl-A&F-FA-Oilex [2)]	60.9	103.2	164.1	60.9	44.1	50.6
		BioPHA-GA-Toa	37.5	56.5	94.0	37.5	20.7	27.3
		BioPHA-GA-Th	94.9	54.9	149.8	94.9	78.1	84.7
		BioPHA-GA-Tey	111.6	54.9	166.5	111.6	94.8	101.4
		BioPHA-GA-Tex	91.3	53.0	144.2	91.3	74.5	81.0
		BioPHA-GA-Texey	108.1	53.0	161.0	108.1	91.3	97.8
		BioPHA-GA-OilTexey [2)]	109.0	62.5	171.5	109.0	92.2	98.8
		BioPHBV-SRI-Tey-1	143.2	52.4	195.5	143.2	132.3	136.5
		BioPHB-SRI-Tey-2	42.8	52.0	94.8	42.8	31.9	36.2
		BioPHA-GA-Fey-1	82.3	42.1	124.4	82.3	65.5	72.1
		BioPHA-GA-Fey-2	33.3	42.1	75.3	33.3	16.5	23.0
		PchemHDPE	76.6	0.0	76.6	61.5	0.0	0.0
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	40.4	64.0	104.4	40.4	17.3	16.4
		BioEthylene-BioEtOH-Anae-GA-Fpv	31.0	61.5	92.5	31.0	7.9	16.9
		PchemEthylene	65.6	0.0	65.6	65.6	42.4	
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	59.5	21.8	81.3	59.5	48.6	52.9
		EL-Sh-pchemEtOH-bioLA-F2	55.6	21.8	77.4	55.6	44.7	48.9
		BioEL-NW-bioEtOH-bioLA-T1	41.3	31.4	72.8	41.3	30.5	34.7
		BioEL-Sh-bioEtOH-bioLA-F1	41.8	37.0	78.8	41.8	30.9	35.1
		BioEL-NW-bioEtOH-bioLA-F2	36.1	29.5	65.7	36.1	25.3	29.5
		BioEL-Sh-bioEtOH-bioLA-F3	43.3	29.6	72.9	43.3	32.4	36.7
		BioEL-Sh-bioEtOH-bioLA-F4	43.2	37.6	80.8	43.2	32.3	36.6
		PchemEthylAcetate	59.3	0.0	59.3	59.3	47.1	51.9
		PchemBenzene	67.7	0.0	67.7	67.7	48.5	56.0
		PchemEGBE	73.3	0.0	73.3	73.3	53.5	61.2
		PchemMEK	92.1	0.0	92.1	92.1	75.7	82.1
		PchemAcetone	63.0	0.0	63.0	63.0	48.8	54.3
	PLA	BioPLA-bioLA-SRI-TpH6cont	60.8	26.3	87.1	60.8	52.2	55.5
		BioPLA-bioLA-SRI-FlowpH	59.9	37.5	97.4	59.9	51.3	54.6
		BioPLA-bioLA-NW-Tu	52.7	26.5	79.2	52.7	44.1	47.5
		BioPLA-bioLA-Sh-Fex	49.3	37.5	86.8	49.3	40.7	44.0
		BioPLA-bioLA-Sh-Fed	52.3	37.5	89.9	52.3	43.8	47.1
		BioPLA-bioLA-Anaer-GA-Fed	41.1	24.4	65.5	41.1	32.6	35.9
		BioPLA-bioLA-NW-Fu	40.1	24.7	64.8	40.1	31.5	34.9
		PchemPET Amorph	80.8	0.0	80.8	80.8	69.9	74.2
		PchemPS	86.7	0.0	86.7	86.7	67.3	74.9
		PchemPE LD	77.8	0.0	77.8	77.8	54.7	63.7
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	65.1	11.0	76.0	65.1	53.8	58.2
		PTT-bioPDO-Anaer-SRI-Tdcont	68.1	13.8	81.9	68.1	56.9	61.3
		PTT-bioPDO-Aer-DP-Tu	63.0	14.6	77.6	63.0	51.8	56.2
		PTT-bioPDO-Aer-GA-Tevbat	67.5	15.6	83.2	67.5	56.3	60.7
		PTT-bioPDO-Aer-GA-Tevcont	61.8	15.6	77.4	61.8	50.6	54.9
		PTT-bioPDO-Aer-GA-FpvH2O	63.9	12.3	76.2	63.9	52.7	57.0
		PTT-bioPDO-Aer-GA-FpvPDO	55.2	12.3	67.5	55.2	44.0	48.4
		PTT-bioPDO-Anaer-Glyc-SRI-Td [3)]	71.1	15.8	86.9	71.1	59.9	64.3
		PTT-bioPDO-Anaer-Glyc-VDI-Td [3)]	71.4	12.4	83.8	71.4	60.1	64.5
		PTT-PchemPDO-Propyl-DP	81.7	0.1	81.8	81.7	70.5	74.9
		PTT-PchemPDO-EO-SRI	73.5	0.1	73.6	73.5	62.3	66.6
		PTT-PchemPDO-EO-Shell	94.6	0.0	94.6	94.6	83.4	87.7
		PTT-PchemPDO-Acro-SRI	85.3	0.1	85.4	85.3	74.1	78.5
		PchemPET Amorph	80.8	0.0	80.8	80.8	69.9	74.2
		PchemNylon-6	120.5	0.0	120.5	120.5	105.6	111.4
		PchemNylon-6,6	138.6	0.0	138.6	138.6	122.9	129.1

[1)] The original process data used refer to the use of potato slurry proteins and potato steam peals (i.e., not for maize starch). Per tonne of hydrogen, around 2 tonnes of potato slurry proteins are required. It depends on the allocation approach how much land this translates to (we did not conduct calculations for land use).

[2)] This process uses fatty acids (FA) as feedstock for PDO, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane). In our calculations we exclusively assumed rapeseed oil with the typical production characteristics in Europe and assuming a price of rapeseed crude oil of 500 EURO/t.

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[*)] Negative emissions = carbon storage

[**)] Product value =Prod. cost + 30% capital charge

Table A10-3b): Energy use for bio-based and equivalent petrochemical-based platform chemicals and products – Sugar from SUGAR CANE

			Non-renewable and renewable energy use on a cradle-to-factory gate basis			Non-renewable energy use on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	Non-renewable energy use	Renewable energy use	Total energy use	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Sugar Cane	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)
Alcohols	Ethanol	BioEtOH-SRI-Td	-13.7	90.5	76.9	-13.7	-27.3	-22.0
		BioEtOH-SRI-Corn-Td [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		BioEtOH-Anaer-GA-Tdcont	-18.7	93.7	75.0	-18.7	-32.3	-27.0
		BioEtOH-Anaer-GA-Fd	-20.5	90.0	69.5	-20.5	-34.1	-28.8
		BioEtOH-Anaer-GA-Fpv	-22.7	90.0	67.4	-22.7	-36.3	-31.0
		BioEtOH-SRI-Stover-Fd [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemEtOH-1 [2)]	63.9	0.0	63.9	63.9	50.2	55.6
		PchemEtOH-2 [2)]	54.2	0.0	54.3	54.2	40.6	45.9
	PDO	BioPDO-Anaer-SRI-Tdcont	14.5	88.8	103.3	14.5	2.9	7.5
		BioPDO-Aer-SRI-Tdcont	14.0	71.3	85.3	14.0	2.5	7.0
		BioPDO-Aer-DP-Tu	-2.0	94.7	92.7	-2.0	-13.6	-9.0
		BioPDO-Aer-GA-Tevbat	6.9	101.7	108.6	6.9	-4.7	-0.2
		BioPDO-Aer-GA-Tevcont	-8.6	101.7	93.0	-8.6	-20.2	-15.7
		BioPDO-Aer-GA-FpvH2O	6.9	79.9	86.8	6.9	-4.6	-0.1
		BioPDO-Aer-GA-FpvPDO	-16.5	79.9	63.4	-16.5	-28.1	-23.6
		BioPDO-Anaer-Glyc-SRI-Tdcont [3)]	62.8	42.7	105.5	62.8	51.2	55.7
		BioPDO-Anaer-Glyc-VDI-Tdbat [3)]	63.5	33.4	96.8	63.5	51.9	56.4
		PchemPDO-Propyl-DP	91.5	0.0	91.5	91.5	79.9	84.4
		PchemPDO-EO-SRI	69.1	0.0	69.1	69.1	57.6	62.1
		PchemPDO-Acro-SRI	101.2	0.0	101.3	101.2	89.7	94.2
	ABE	BioABE-Anaer-GA-Tdcont	7.4	124.8	132.2	7.4	-9.2	-2.7
		BioABE-Anaer-GA-Tgscont	0.7	124.8	125.5	0.7	-15.9	-9.4
		BioABE-Anaer-GA-Fdm	-18.5	104.8	86.4	-18.5	-35.0	-28.6
		BioABE-Anaer-GA-Fmd	-40.9	104.8	64.0	-40.9	-57.5	-51.0
		BioABE-Anaer-GA-Fpv	-39.6	104.8	65.2	-39.6	-56.2	-49.7
		BioABE-Anaer-GA-Fgs	-29.4	104.8	75.5	-29.4	-45.9	-39.5
		PchemButanol	69.3	0.0	69.3	69.3	52.7	59.2
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	106.3	85.6	191.9	106.3	99.1	101.9
		BioAcet-Anaer-GA-Ted	70.7	84.8	155.5	70.7	63.6	66.4
		BioAcet-Anaer-GA-FexTOPO	36.3	46.9	83.2	36.3	29.1	31.9
		BioAcet-Anaer-GA-FexDIPE	43.3	47.8	91.1	43.3	36.2	39.0
		BioAcet-Anaer-GA-FedexDIPE	17.6	47.3	64.9	17.6	10.4	13.2
		BioAcet-Anaer-GA-Fed	22.5	47.1	69.6	22.5	15.3	18.1
		PchemAceticAcid	55.5	0.0	55.5	55.5	48.6	51.3
	Acrylic acid	BioAcryl-Anaer-GA-Fex	4.4	58.1	62.5	4.4	-4.2	-0.8
		PchemAcrylicAcid	47.1	0.0	47.1	47.1	38.5	41.9
	Lactic acid	BioLA-SRI-TpH6cont	15.7	48.6	64.3	15.7	8.6	11.4
		BioLA-SRI-FlowpH	15.0	57.4	72.4	15.0	7.9	10.7
		BioLA-NW-Tu	9.0	49.3	58.3	9.0	1.9	4.6
		BioLA-Sh-Fex	6.7	57.4	64.1	6.7	-0.4	2.4
		BioLA-Sh-Fed	9.1	57.4	66.5	9.1	2.0	4.8
		BioLA-Anaer-GA-Fed	1.8	45.9	47.7	1.8	-5.4	-2.6
		BioLA-NW-Fu	-1.5	46.4	45.0	-1.5	-8.6	-5.8
	Succinic acid	BioSA-Anaer-GA-Tc	44.9	63.9	108.9	44.9	38.8	41.2
		BioSA-Anaer-GA-Ted	5.4	62.5	67.9	5.4	-0.7	1.7
		BioSA-Aer-SRI-Fed	26.8	45.3	72.2	26.8	20.7	23.1
		BioSA-Anaer-GA-Fcrx	13.6	46.2	59.8	13.6	7.4	9.8
		BioSA-Anaer-GA-Fc	30.7	40.9	71.6	30.7	24.6	26.9
		BioSA-Anaer-GA-Fed	9.1	45.1	54.2	9.1	3.0	5.4
		PchemMaleicAnhydride	67.7	1.2	69.0	67.7	61.9	64.2
		PchemSA-MalAnhydr	96.3	1.4	97.7	96.3	90.1	92.5
	Adipic acid	BioAdip-Aer-GA-Tc	85.7	241.6	327.3	85.7	76.8	80.3
		BioAdip-Aer-GA-Fc	19.4	88.6	107.9	19.4	10.5	13.9
		BioAdip-Aer-GA-Fed	3.2	90.4	93.7	3.2	-5.6	-2.2
		PchemAdipicAcid	85.5	0.0	85.5	85.5	76.6	80.1
	Citric acid	BioCit-Aer-SRI-Tevc [4)]	73.7	0.6	74.3	73.7	68.9	70.8
		BioCit-Aer-SRI-Tix	26.2	107.8	134.0	26.2	21.4	23.3
		BioCit-Aer-GA-Tpc	29.3	149.3	178.6	29.3	24.6	26.4
		BioCit-Aer-GA-Fc	1.7	44.9	46.6	1.7	-3.1	-1.3

[1)] The original process data used cover all steps starting with the intake of corn (for BioEtOH-SRI-Corn-Td) and corn stover (for BioEtOH-SRI-Stover-Fd). For this reason results can only be presented for these two feedstock types (see tables for maize starch and lignocellulosics).

[2)] Dataset PchemEtOH-1 is based on SRI data while dataset PchemEtOH-2 originates from the project C-STREAMS (Patel et al, 1999).

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[4)] The original process data used refer to the use of cane molasses. For this reason results are only presented for sugar cane as feedstock type and *not* for maize starch and lignocellulosics. Per tonne of citric acid, 2.6-2.8 tonnes of cane molasses are required. It depends on the allocation approach how much land this translates to (no allocation has been performed here).

			Non-renewable and renewable energy use on a cradle-to-factory gate basis			Non-renewable energy use on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	Non-renewable energy use	Renewable energy use	Total energy use	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Sugar Cane	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	-5.7	108.1	102.4	-5.7	-20.4	-14.7
		PchemCapro	117.1	0.0	117.1	117.1	102.4	108.1
	Lysine	BioLys-Aer-SRI-Tix	136.8	118.1	254.8	136.8	123.9	128.9
		BioLys-Aer-SRI-Tsp	4.8	134.5	139.3	4.8	-8.1	-3.0
		BioLys-Aer-GA-Tix	82.8	190.4	273.2	82.8	70.0	75.0
		BioLys-Aer-GA-Fad	70.7	133.0	203.6	70.7	57.8	62.8
H_2	Hydrogen	BioH2-A&F-gs [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemH2	180.0	0.0	180.0			
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	17.2	125.9	143.1	17.2	0.4	6.9
		BioPHAmcl-A&F-FA-Oilex [2)]	60.9	103.2	164.1	60.9	44.1	50.6
		BioPHA-GA-Toa	-23.9	135.7	111.8	-23.9	-40.7	-34.1
		BioPHA-GA-Th	34.9	132.2	167.2	34.9	18.1	24.7
		BioPHA-GA-Tey	51.6	132.2	183.8	51.6	34.8	41.4
		BioPHA-GA-Tex	33.4	127.6	161.0	33.4	16.6	23.1
		BioPHA-GA-Texey	50.2	127.6	177.8	50.2	33.4	39.9
		BioPHA-GA-OilTexey [2)]	109.0	62.5	171.5	109.0	92.2	98.8
		BioPHBV-SRI-Tey-1	86.2	125.9	212.0	86.2	75.3	79.5
		BioPHB-SRI-Tey-2	-14.2	125.5	111.3	-14.2	-25.1	-20.8
		BioPHA-GA-Fey-1	36.3	101.4	137.7	36.3	19.5	26.1
		BioPHA-GA-Fey-2	-12.8	101.4	88.7	-12.8	-29.6	-23.0
		PchemHDPE	76.6	0.0	76.6	61.5	0.0	0.0
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	-29.9	154.6	124.7	-29.9	-53.0	16.4
		BioEthylene-BioEtOH-Anae-GA-Fpv	-36.5	148.5	112.1	-36.5	-59.6	-50.6
		PchemEthylene	65.6	0.0	65.6	65.6	42.4	
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	43.3	42.7	86.0	43.3	32.5	36.7
		EL-Sh-pchemEtOH-bioLA-F2	39.4	42.7	82.1	39.4	28.5	32.7
		BioEL-NW-bioEtOH-bioLA-T1	7.3	75.3	82.6	7.3	-3.6	0.7
		BioEL-Sh-bioEtOH-bioLA-F1	8.9	79.4	88.3	8.9	-2.0	2.2
		BioEL-NW-bioEtOH-bioLA-F2	3.8	71.2	75.0	3.8	-7.1	-2.9
		BioEL-Sh-bioEtOH-bioLA-F3	27.1	50.4	77.6	27.1	16.3	20.5
		BioEL-Sh-bioEtOH-bioLA-F4	9.6	80.9	90.5	9.6	-1.2	3.0
		PchemEthylAcetate	59.3	0.0	59.3	59.3	47.1	51.9
		PchemBenzene	67.7	0.0	67.7	67.7	48.5	56.0
		PchemEGBE	73.3	0.0	73.3	73.3	53.5	61.2
		PchemMEK	92.1	0.0	92.1	92.1	75.7	82.1
		PchemAcetone	63.0	0.0	63.0	63.0	48.8	54.3
	PLA	BioPLA-bioLA-SRI-TpH6cont	32.9	62.2	95.1	32.9	24.4	27.7
		BioPLA-bioLA-SRI-FlowpH	32.0	73.4	105.5	32.0	23.4	26.8
		BioPLA-bioLA-NW-Tu	24.3	63.1	87.4	24.3	15.7	19.1
		BioPLA-bioLA-Sh-Fex	21.4	73.4	94.9	21.4	12.8	16.2
		BioPLA-bioLA-Sh-Fed	24.5	73.4	97.9	24.5	15.9	19.3
		BioPLA-bioLA-Anaer-GA-Fed	14.5	58.7	73.2	14.5	5.9	9.2
		BioPLA-bioLA-NW-Fu	13.2	59.4	72.6	13.2	4.6	8.0
		PchemPET Amorph	80.8	0.0	80.8	80.8	69.9	74.2
		PchemPS	86.7	0.0	86.7	86.7	67.3	74.9
		PchemPE LD	77.8	0.0	77.8	77.8	54.7	63.7
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	53.1	26.4	79.5	53.1	41.9	46.2
		PTT-bioPDO-Anaer-SRI-Tdcont	53.3	32.9	86.2	53.3	42.1	46.4
		PTT-bioPDO-Aer-DP-Tu	47.2	35.1	82.2	47.2	35.9	40.3
		PTT-bioPDO-Aer-GA-Tevbat	50.5	37.6	88.1	50.5	39.2	43.6
		PTT-bioPDO-Aer-GA-Tevcont	44.7	37.6	82.4	44.7	33.5	37.9
		PTT-bioPDO-Aer-GA-FpvH2O	50.5	29.6	80.1	50.5	39.3	43.6
		PTT-bioPDO-Aer-GA-FpvPDO	41.8	29.6	71.4	41.8	30.6	35.0
		PTT-bioPDO-Anaer-Glyc-SRI-Tdcont [3)]	71.1	15.8	86.9	71.1	59.9	64.3
		PTT-bioPDO-Anaer-Glyc-VDI-Tdbat [3)]	71.4	12.4	83.8	71.4	60.1	64.5
		PTT-PchemPDO-Propyl-DP	81.7	0.1	81.8	81.7	70.5	74.9
		PTT-PchemPDO-EO-SRI	73.5	0.1	73.6	73.5	62.3	66.6
		PTT-PchemPDO-EO-Shell	94.6	0.0	94.6	94.6	83.4	87.7
		PTT-PchemPDO-Acro-SRI	85.3	0.1	85.4	85.3	74.1	78.5
		PchemPET Amorph	80.8	0.0	80.8	80.8	69.9	74.2
		PchemNylon-6	120.5	0.0	120.5	120.5	105.6	111.4
		PchemNylon-6,6	138.6	0.0	138.6	138.6	122.9	129.1

[1)] The original process data used refer to the use of potato slurry proteins and potato steam peals. These results are reported in the table for maize starch.

[2)] This process uses fatty acids (FA) as feedstock for PDO, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane). In our calculations we exclusively assumed rapeseed oil with the typical production characteristics in Europe and assuming a price of rapeseed crude oil of 500 EURO/t.

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[*)] Negative emissions = carbon storage

[**)] Product value =Prod. cost + 30% capital charge

Table A10-3c): Energy use for bio-based and equivalent petrochemical-based platform chemicals and products – Sugar from LIGNOCELLULOSE

			Non-renewable and renewable energy use on a cradle-to-factory gate basis			Non-renewable energy use on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	Non-renewable energy use	Renewable energy use	Total energy use	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Lignocellulosics	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)
Alcohols	Ethanol	BioEtOH-SRI-Td	4.4	63.6	68.0	4.4	-9.2	-3.9
		BioEtOH-SRI-Corn-Td [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		BioEtOH-Anaer-GA-Tdcont	0.2	65.5	65.7	0.2	-13.4	-8.1
		BioEtOH-Anaer-GA-Fd	-2.3	62.9	60.6	-2.3	-16.0	-10.7
		BioEtOH-Anaer-GA-Fpv	-4.5	62.9	58.4	-4.5	-18.1	-12.8
		BioEtOH-SRI-Stover-Fd	22.8	56.1	78.9	22.8	9.2	14.5
		PchemEtOH-1 [2)]	63.9	0.0	63.9	63.9	50.2	55.6
		PchemEtOH-2 [2)]	54.2	0.0	54.3	54.2	40.6	45.9
	PDO	BioPDO-Anaer-SRI-Tdcont	32.3	62.3	94.6	32.3	20.7	25.2
		BioPDO-Aer-SRI-Tdcont	28.4	49.9	78.3	28.4	16.8	21.3
		BioPDO-Aer-DP-Tu	17.1	66.3	83.3	17.1	5.5	10.0
		BioPDO-Aer-GA-Tevbat	27.4	71.1	98.5	27.4	15.8	20.3
		BioPDO-Aer-GA-Tevcont	11.9	71.1	83.0	11.9	0.3	4.8
		BioPDO-Aer-GA-FpvH2O	23.1	55.9	78.9	23.1	11.5	16.0
		BioPDO-Aer-GA-FpvPDO	-0.4	55.9	55.5	-0.4	-12.0	-7.5
		BioPDO-Anaer-Glyc-SRI-Tdcont [3)]	62.8	42.7	105.5	62.8	51.2	55.7
		BioPDO-Anaer-Glyc-VDI-Tdbat [3)]	63.5	33.4	96.8	63.5	51.9	56.4
		PchemPDO-Propyl-DP	91.5	0.0	91.5	91.5	79.9	84.4
		PchemPDO-EO-SRI	69.1	0.0	69.1	69.1	57.6	62.1
		PchemPDO-Acro-SRI	101.2	0.0	101.3	101.2	89.7	94.2
	ABE	BioABE-Anaer-GA-Tdcont	32.5	87.4	119.9	32.5	15.9	22.4
		BioABE-Anaer-GA-Tgscont	25.8	87.4	113.1	25.8	9.2	15.7
		BioABE-Anaer-GA-Fdm	2.6	73.4	76.0	2.6	-13.9	-7.5
		BioABE-Anaer-GA-Fmd	-19.8	73.4	53.6	-19.8	-36.4	-29.9
		BioABE-Anaer-GA-Fpv	-18.5	73.4	54.9	-18.5	-35.1	-28.6
		BioABE-Anaer-GA-Fgs	-8.3	73.4	65.1	-8.3	-24.8	-18.4
		PchemButanol	69.3	0.0	69.3	69.3	52.7	59.2
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	123.4	60.1	183.5	123.4	116.3	119.0
		BioAcet-Anaer-GA-Ted	87.7	59.5	147.2	87.7	80.5	83.3
		BioAcet-Anaer-GA-FexTOPO	45.7	32.9	78.6	45.7	38.5	41.3
		BioAcet-Anaer-GA-FexDIPE	52.9	33.5	86.4	52.9	45.8	48.5
		BioAcet-Anaer-GA-FedexDIPE	27.0	33.2	60.2	27.0	19.9	22.7
		BioAcet-Anaer-GA-Fed	31.9	33.1	64.9	31.9	24.7	27.5
		PchemAceticAcid	55.5	0.0	55.5	55.5	48.6	51.3
	Acrylic acid	BioAcryl-Anaer-GA-Fex	16.1	40.6	56.7	16.1	7.5	10.9
		PchemAcrylicAcid	47.1	0.0	47.1	47.1	38.5	41.9
	Lactic acid	BioLA-SRI-TpH6cont	25.4	34.2	59.6	25.4	18.2	21.0
		BioLA-SRI-FlowpH	24.7	43.0	67.6	24.7	17.5	20.3
		BioLA-NW-Tu	18.8	34.6	53.4	18.8	11.7	14.5
		BioLA-Sh-Fex	16.4	43.0	59.3	16.4	9.2	12.0
		BioLA-Sh-Fed	18.8	43.0	61.8	18.8	11.7	14.4
		BioLA-Anaer-GA-Fed	11.0	32.1	43.1	11.0	3.9	6.7
		BioLA-NW-Fu	7.9	32.5	40.4	7.9	0.7	3.5
	Succinic acid	BioSA-Anaer-GA-Tc	54.5	49.7	104.2	54.5	48.4	50.8
		BioSA-Anaer-GA-Ted	15.0	48.2	63.2	15.0	8.8	11.2
		BioSA-Aer-SRI-Fed	35.1	32.9	68.1	35.1	29.0	31.4
		BioSA-Anaer-GA-Fcrx	22.0	33.7	55.7	22.0	15.8	18.2
		BioSA-Anaer-GA-Fc	37.8	30.2	68.1	37.8	31.7	34.1
		BioSA-Anaer-GA-Fed	17.5	32.6	50.1	17.5	11.3	13.7
		PchemMaleicAnhydride	67.7	1.2	69.0	67.7	61.9	64.2
		PchemSA-MalAnhydr	96.3	1.4	97.7	96.3	90.1	92.5
	Adipic acid	BioAdip-Aer-GA-Tc	134.4	169.0	303.4	134.4	125.5	129.0
		BioAdip-Aer-GA-Fc	37.2	61.9	99.2	37.2	28.3	31.8
		BioAdip-Aer-GA-Fed	21.5	63.2	84.7	21.5	12.6	16.1
		PchemAdipicAcid	85.5	0.0	85.5	85.5	76.6	80.1
	Citric acid	BioCit-Aer-SRI-Tevc [4)]	73.7	0.6	74.3	73.7	68.9	70.8
		BioCit-Aer-SRI-Tix	47.8	75.5	123.4	47.8	43.1	44.9
		BioCit-Aer-GA-Tpc	59.4	104.5	163.9	59.4	54.6	56.5
		BioCit-Aer-GA-Fc	10.7	31.4	42.1	10.7	5.9	7.8

[1)] The original process data used cover all steps starting with the intake of corn. The results are therefore given in the table for starch maize starch.

[2)] Dataset PchemEtOH-1 is based on SRI data while dataset PchemEtOH-2 originates from the project C-STREAMS (Patel et al, 1999).

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[4)] The original process data used refer to the use of cane molasses. For this reason results are only presented for sugar cane as feedstock type and *not* for maize starch and lignocellulosics.

			Non-renewable and renewable energy use on a cradle-to-factory gate basis			Non-renewable energy use on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	Non-renewable energy use	Renewable energy use	Total energy use	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Lignocellulosics	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)	(GJ/t)
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	16.0	75.6	91.6	16.0	1.4	7.1
		PchemCapro	117.1	0.0	117.1	117.1	102.4	108.1
	Lysine	BioLys-Aer-SRI-Tix	160.0	83.4	243.4	160.0	147.1	152.2
		BioLys-Aer-SRI-Tsp	31.9	94.0	125.9	31.9	19.0	24.1
		BioLys-Aer-GA-Tix	120.9	133.5	254.5	120.9	108.1	113.1
		BioLys-Aer-GA-Fad	97.5	93.0	190.4	97.5	84.6	89.6
H_2	Hydrogen	BioH2-A&F-gs [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemH2	180.0	0.0	180.0			
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	38.3	94.4	132.7	38.3	21.5	28.0
		BioPHAmcl-A&F-FA-Oilex [2)]	60.9	103.2	164.1	60.9	44.1	50.6
		BioPHA-GA-Toa	3.4	95.0	98.4	3.4	-13.4	-6.9
		BioPHA-GA-Th	61.6	92.5	154.1	61.6	44.8	51.3
		BioPHA-GA-Tey	78.2	92.5	170.7	78.2	61.4	68.0
		BioPHA-GA-Tex	59.1	89.3	148.4	59.1	42.3	48.8
		BioPHA-GA-Texey	75.9	89.3	165.2	75.9	59.1	65.6
		BioPHA-GA-OilTexey [2)]	109.0	62.5	171.5	109.0	92.2	98.8
		BioPHBV-SRI-Tey-1	111.5	88.1	199.6	111.5	100.6	104.8
		BioPHB-SRI-Tey-2	11.1	87.7	98.8	11.1	0.2	4.5
		BioPHA-GA-Fey-1	56.7	71.0	127.7	56.7	40.0	46.5
		BioPHA-GA-Fey-2	7.7	71.0	78.6	7.7	-9.1	-2.6
		PchemHDPE	76.6	0.0	76.6	61.5	0.0	0.0
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	1.3	108.1	109.4	1.3	-21.8	16.4
		BioEthylene-BioEtOH-Anae-GA-Fpv	-6.5	103.8	97.3	-6.5	-29.6	-20.6
		PchemEthylene	65.6	0.0	65.6	65.6	42.4	
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	50.5	32.0	82.5	50.5	39.6	43.9
		EL-Sh-pchemEtOH-bioLA-F2	46.6	32.0	78.5	46.6	35.7	39.9
		BioEL-NW-bioEtOH-bioLA-T1	22.4	52.8	75.2	22.4	11.5	15.8
		BioEL-Sh-bioEtOH-bioLA-F3	34.3	39.7	74.0	34.3	23.4	27.7
		BioEL-Sh-bioEtOH-bioLA-F4	24.5	58.7	83.2	24.5	13.7	17.9
		PchemEthylAcetate	59.3	0.0	59.3	59.3	47.1	51.9
		PchemBenzene	67.7	0.0	67.7	67.7	48.5	56.0
		PchemEGBE	73.3	0.0	73.3	73.3	53.5	61.2
		PchemMEK	92.1	0.0	92.1	92.1	75.7	82.1
		PchemAcetone	63.0	0.0	63.0	63.0	48.8	54.3
	PLA	BioPLA-bioLA-SRI-TpH6cont	45.3	43.8	89.1	45.3	36.7	40.1
		BioPLA-bioLA-SRI-FlowpH	44.4	55.0	99.4	44.4	35.8	39.1
		BioPLA-bioLA-NW-Tu	36.9	44.3	81.2	36.9	28.3	31.7
		BioPLA-bioLA-Sh-Fex	33.8	55.0	88.8	33.8	25.2	28.5
		BioPLA-bioLA-Sh-Fed	36.9	55.0	91.9	36.9	28.3	31.6
		BioPLA-bioLA-Anaer-GA-Fed	26.3	41.1	67.4	26.3	17.7	21.1
		BioPLA-bioLA-NW-Fu	25.1	41.6	66.7	25.1	16.6	19.9
		PchemPET Amorph	80.8	0.0	80.8	80.8	69.9	74.2
		PchemPS	86.7	0.0	86.7	86.7	67.3	74.9
		PchemPE LD	77.8	0.0	77.8	77.8	54.7	63.7
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	58.4	18.5	76.9	58.4	47.2	51.5
		PTT-bioPDO-Anaer-SRI-Tdcont	59.9	23.1	83.0	59.9	48.6	53.0
		PTT-bioPDO-Aer-DP-Tu	54.2	24.5	78.8	54.2	43.0	47.4
		PTT-bioPDO-Aer-GA-Tevbat	58.0	26.3	84.4	58.0	46.8	51.2
		PTT-bioPDO-Aer-GA-Tevcont	52.3	26.3	78.6	52.3	41.1	45.4
		PTT-bioPDO-Aer-GA-FpvH2O	56.4	20.7	77.1	56.4	45.2	49.6
		PTT-bioPDO-Aer-GA-FpvPDO	47.8	20.7	68.5	47.8	36.5	40.9
		PTT-bioPDO-Anaer-Glyc-SRI-Tdcont [3)]	71.1	15.8	86.9	71.1	59.9	64.3
		PTT-bioPDO-Anaer-Glyc-VDI-Tdbat [3)]	71.4	12.4	83.8	71.4	60.1	64.5
		PTT-PchemPDO-Propyl-DP	81.7	0.1	81.8	81.7	70.5	74.9
		PTT-PchemPDO-EO-SRI	73.5	0.1	73.6	73.5	62.3	66.6
		PTT-PchemPDO-EO-Shell	94.6	0.0	94.6	94.6	83.4	87.7
		PTT-PchemPDO-Acro-SRI	85.3	0.1	85.4	85.3	74.1	78.5
		PchemPET Amorph	80.8	0.0	80.8	80.8	69.9	74.2
		PchemNylon-6	120.5	0.0	120.5	120.5	105.6	111.4
		PchemNylon-6,6	138.6	0.0	138.6	138.6	122.9	129.1

[1)] The original process data used refer to the use of potato slurry proteins and potato steam peals. These results are reported in the table for maize starch. It depends on the allocation approach how much land this translates to (we did not conduct calculations for land use).

[2)] This process uses fatty acids (FA) as feedstock for PDO, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane). In our calculations we exclusively assumed rapeseed oil with the typical production characteristics in Europe and assuming a price of rapeseed crude oil of 500 EURO/t.

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[*)] Negative emissions = carbon storage

[**)] Product value =Prod. cost + 30% capital charge

Table A10-4a): GHG emissions for bio-based and equivalent petrochemical-based platform chemicals and products – Sugar from STARCH

			GHG emissions			GHG emissions on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	GHG emissions cradle-to-grave	Renew. C stored in product (CO2 eq.)	GHG emissions cradle-to-factory gate	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Maize Starch	(t CO_2eq./t)	(t CO_2/t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)
Alcohols	Ethanol	BioEtOH-SRI-Td	1.7	-1.9	-0.2	1.7	1.0	1.3
		BioEtOH-SRI-Corn-Td	2.1	-1.9	0.2	2.1	1.4	1.7
		BioEtOH-Anaer-GA-Tdcont	1.5	-1.9	-0.4	1.5	0.8	1.1
		BioEtOH-Anaer-GA-Fd	1.3	-1.9	-0.6	1.3	0.6	0.9
		BioEtOH-Anaer-GA-Fpv	1.2	-1.9	-0.7	1.2	0.5	0.8
		BioEtOH-SRI-Stover-Fd [1]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemEtOH-1 [2]	2.0	0.0	2.0	3.9	3.2	3.5
		PchemEtOH-2 [2]	1.3	0.0	1.3	3.2	2.5	2.8
	PDO	BioPDO-Anaer-SRI-Tdcont	3.3	-1.7	1.5	3.3	2.7	2.9
		BioPDO-Aer-SRI-Tdcont	2.8	-1.7	1.1	2.8	2.2	2.5
		BioPDO-Aer-DP-Tu	2.3	-1.7	0.5	2.3	1.7	1.9
		BioPDO-Aer-GA-Tevbat	3.0	-1.7	1.3	3.0	2.4	2.7
		BioPDO-Aer-GA-Tevcont	2.3	-1.7	0.5	2.3	1.7	1.9
		BioPDO-Aer-GA-FpvH2O	2.7	-1.7	0.9	2.7	2.1	2.3
		BioPDO-Aer-GA-FpvPDO	1.2	-1.7	-0.5	1.2	0.6	0.9
		BioPDO-Anaer-Glyc-SRI-Tdcont [3]	3.4	-1.7	1.7	3.4	2.9	3.1
		BioPDO-Anaer-Glyc-VDI-Tdbat [3]	3.5	-1.7	1.8	3.5	2.9	3.2
		PchemPDO-Propyl-DP	3.6	0.0	3.6	5.4	4.8	5.0
		PchemPDO-EO-SRI	2.3	0.0	2.3	4.1	3.5	3.7
		PchemPDO-Acro-SRI	4.4	0.0	4.4	6.1	5.5	5.8
	ABE	BioABE-Anaer-GA-Tdcont	3.5	-2.4	1.1	3.5	2.6	3.0
		BioABE-Anaer-GA-Tgscont	3.0	-2.4	0.7	3.0	2.2	2.5
		BioABE-Anaer-GA-Fdm	1.7	-2.4	-0.6	1.7	0.9	1.3
		BioABE-Anaer-GA-Fmd	0.4	-2.4	-2.0	0.4	-0.5	-0.1
		BioABE-Anaer-GA-Fpv	0.4	-2.4	-1.9	0.4	-0.4	-0.1
		BioABE-Anaer-GA-Fgs	1.0	-2.4	-1.3	1.0	0.2	0.5
		PchemButanol	1.9	0.0	1.9	4.3	3.4	3.8
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	8.1	-1.5	6.6	8.1	7.7	7.9
		BioAcet-Anaer-GA-Ted	5.7	-1.5	4.2	5.7	5.3	5.5
		BioAcet-Anaer-GA-FexTOPO	3.5	-1.5	2.1	3.5	3.2	3.3
		BioAcet-Anaer-GA-FexDIPE	3.9	-1.5	2.5	3.9	3.6	3.7
		BioAcet-Anaer-GA-FedexDIPE	2.1	-1.5	0.7	2.1	1.8	1.9
		BioAcet-Anaer-GA-Fed	2.4	-1.5	1.0	2.4	2.0	2.2
		PchemAceticAcid	1.8	0.0	1.8	3.3	2.9	3.1
	Acrylic acid	BioAcryl-Anaer-GA-Fex	2.0	-1.8	0.2	2.0	1.5	1.7
		PchemAcrylicAcid	1.7	0.0	1.7	3.5	3.1	3.2
	Lactic acid	BioLA-SRI-TpH6cont	2.7	-1.5	1.2	2.7	2.3	2.5
		BioLA-SRI-FlowpH	2.4	-1.5	0.9	2.4	2.0	2.1
		BioLA-NW-Tu	2.0	-1.5	0.5	2.0	1.6	1.8
		BioLA-Sh-Fex	1.9	-1.5	0.4	1.9	1.5	1.7
		BioLA-Sh-Fed	1.8	-1.5	0.4	1.8	1.5	1.6
		BioLA-Anaer-GA-Fed	1.2	-1.5	-0.3	1.2	0.8	1.0
		BioLA-NW-Fu	1.2	-1.5	-0.2	1.2	0.9	1.0
	Succinic acid	BioSA-Anaer-GA-Tc	4.6	-1.5	3.1	4.6	4.3	4.4
		BioSA-Anaer-GA-Ted	2.3	-1.5	0.8	2.3	2.0	2.1
		BioSA-Aer-SRI-Fed	2.8	-1.5	1.3	2.8	2.4	2.6
		BioSA-Anaer-GA-Fcrx	2.0	-1.5	0.5	2.0	1.7	1.8
		BioSA-Anaer-GA-Fc	2.9	-1.5	1.4	2.9	2.6	2.7
		BioSA-Anaer-GA-Fed	1.8	-1.5	0.3	1.8	1.5	1.6
		PchemMaleicAnhydride	5.0	0.0	5.0	6.8	6.5	6.6
		PchemSA-MalAnhydr	7.1	0.0	7.1	8.6	8.3	8.4
	Adipic acid	BioAdip-Aer-GA-Tc	11.0	-1.8	9.2	11.0	10.5	10.7
		BioAdip-Aer-GA-Fc	3.6	-1.8	1.8	3.6	3.1	3.3
		BioAdip-Aer-GA-Fed	2.5	-1.8	0.7	2.5	2.0	2.2
		PchemAdipicAcid	4.0	0.0	4.0	5.8	5.3	5.5
	Citric acid	BioCit-Aer-SRI-Tevc [4]	4.3	-1.4	2.9	4.3	4.1	4.2
		BioCit-Aer-SRI-Tix	4.5	-1.4	3.1	4.5	4.3	4.4
		BioCit-Aer-GA-Tpc	4.6	-1.4	3.2	4.6	4.4	4.5
		BioCit-Aer-GA-Fc	1.3	-1.4	0.0	1.3	1.1	1.2

[1] The original process data used cover all steps starting with the intake of corn stover (for BioEtOH-SRI-Stover-Fd). The results are therefore given in the table for lignocellulosic inputs.

[2] Dataset PchemEtOH-1 is based on SRI data while dataset PchemEtOH-2 originates from the project C-STREAMS (Patel et al, 1999).

[3] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[4] The original process data used refer to the use of cane molasses. For this reason results are only presented for sugar cane as feedstock type and *not* for maize starch and lignocellulosics.

		Production system	GHG emissions			GHG emissions on a cradle-to-grave basis for three different end-of-life scenarios		
			GHG emissions cradle-to-grave	Renew. C stored in product (CO2 eq.)	GHG emissions cradle-to-factory gate	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Maize Starch	(t CO_2eq./t)	(t CO_2/t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	2.4	-2.3	0.1	2.4	1.7	2.0
		PchemCapro	5.3	0.0	5.3	7.6	6.8	7.1
	Lysine	BioLys-Aer-SRI-Tix	10.3	-1.8	8.5	10.3	9.6	9.9
		BioLys-Aer-SRI-Tsp	3.7	-1.8	1.9	3.7	3.0	3.3
		BioLys-Aer-GA-Tix	8.1	-1.8	6.3	8.1	7.5	7.8
		BioLys-Aer-GA-Fad	6.7	-1.8	4.9	6.7	6.1	6.3
H_2	Hydrogen	BioH2-A&F-gs [1)]	0.7	0.0	0.7			
		PchemH2						
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	4.6	-2.6	2.0	4.6	3.7	4.1
		BioPHAmcl-A&F-FA-Oilex [2)]	7.6	-2.6	5.0	7.6	6.7	7.1
		BioPHA-GA-Toa	1.9	-2.6	-0.7	1.9	1.0	1.4
		BioPHA-GA-Th	5.7	-2.6	3.1	5.7	4.9	5.2
		BioPHA-GA-Tey	6.7	-2.6	4.2	6.7	5.9	6.2
		BioPHA-GA-Tex	5.6	-2.6	3.0	5.6	4.7	5.1
		BioPHA-GA-Texey	6.6	-2.6	4.0	6.6	5.7	6.1
		BioPHA-GA-OilTexey [2)]	9.5	-2.6	6.9	9.5	8.6	9.0
		BioPHBV-SRI-Tey-1	7.5	-2.0	5.4	7.5	6.9	7.2
		BioPHB-SRI-Tey-2	2.7	-2.0	0.7	2.7	2.1	2.4
		BioPHA-GA-Fey-1	2.9	-2.6	0.4	2.9	2.1	2.4
		BioPHA-GA-Fey-2	1.9	-2.6	-0.6	1.9	1.1	1.4
		PchemHDPE	1.6	0.0	1.6	4.7	3.5	4.0
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	2.5	-3.1	-0.6	2.5	1.3	1.8
		BioEthylene-BioEtOH-Anae-GA-Fpv	2.0	-3.1	-1.2	2.0	0.8	1.3
		PchemEthylene	1.3	0.0	1.3	4.4	3.2	3.7
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	3.1	-1.1	2.0	3.9	3.3	3.5
		EL-Sh-pchemEtOH-bioLA-F2	2.8	-1.1	1.7	3.6	3.0	3.3
		BioEL-NW-bioEtOH-bioLA-T1	2.6	-1.9	0.7	2.6	2.0	2.2
		BioEL-Sh-bioEtOH-bioLA-F1	2.8	-1.9	0.9	2.8	2.2	2.5
		BioEL-NW-bioEtOH-bioLA-F2	2.0	-1.9	0.2	2.0	1.5	1.7
		BioEL-Sh-bioEtOH-bioLA-F3	2.3	-1.9	0.5	2.3	1.8	2.0
		BioEL-Sh-bioEtOH-bioLA-F4	2.9	-1.9	1.0	2.9	2.3	2.6
		PchemEthylAcetate	1.9	0.0	1.9	3.9	3.3	3.5
		PchemBenzene	1.5	0.0	1.5	4.9	3.9	4.3
		PchemEGBE	1.8	0.0	1.8	4.0	3.0	3.4
		PchemMEK	3.3	0.0	3.3	5.7	4.8	5.2
		PchemAcetone	1.9	0.0	1.9	4.2	3.4	3.7
	PLA	BioPLA-bioLA-SRI-TpH6cont	4.2	-1.8	2.4	4.2	3.8	3.9
		BioPLA-bioLA-SRI-FlowpH	3.7	-1.8	1.9	3.7	3.3	3.5
		BioPLA-bioLA-NW-Tu	3.3	-1.8	1.4	3.3	2.8	3.0
		BioPLA-bioLA-Sh-Fex	3.2	-1.8	1.3	3.2	2.7	2.9
		BioPLA-bioLA-Sh-Fed	3.1	-1.8	1.2	3.1	2.6	2.8
		BioPLA-bioLA-Anaer-GA-Fed	2.2	-1.8	0.4	2.2	1.8	2.0
		BioPLA-bioLA-NW-Fu	2.5	-1.8	0.7	2.5	2.1	2.3
		PchemPET Amorph	3.3	0.0	3.3	5.6	5.0	5.3
		PchemPS	2.6	0.0	2.6	6.0	5.0	5.4
		PchemPE LD	1.9	0.0	1.9	5.0	3.8	4.3
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	3.0	-0.6	2.4	4.7	4.1	4.4
		PTT-bioPDO-Anaer-SRI-Tdcont	3.2	-0.6	2.5	4.9	4.3	4.5
		PTT-bioPDO-Aer-DP-Tu	2.8	-0.6	2.2	4.5	3.9	4.2
		PTT-bioPDO-Aer-GA-Tevbat	3.1	-0.6	2.4	4.8	4.2	4.4
		PTT-bioPDO-Aer-GA-Tevcont	2.8	-0.6	2.2	4.5	3.9	4.2
		PTT-bioPDO-Aer-GA-FpvH2O	2.9	-0.6	2.3	4.7	4.1	4.3
		PTT-bioPDO-Aer-GA-FpvPDO	2.4	-0.6	1.8	4.1	3.5	3.8
		PTT-bioPDO-Anaer-Glyc-SRI-Td [3)]	3.2	-0.6	2.6	4.9	4.4	4.6
		PTT-bioPDO-Anaer-Glyc-VDI-Td [3)]	3.3	-0.6	2.6	5.0	4.4	4.6
		PTT-PchemPDO-Propyl-DP	3.3	0.0	3.3	5.7	5.1	5.3
		PTT-PchemPDO-EO-SRI	2.8	0.0	2.8	5.2	4.6	4.8
		PTT-PchemPDO-EO-Shell	4.1	0.0	4.1	4.1	3.5	3.8
		PTT-PchemPDO-Acro-SRI	3.6	0.0	3.6	5.9	5.3	5.6
		PchemPET Amorph	3.3	0.0	3.3	5.6	5.0	5.3
		PchemNylon-6	5.5	0.0	5.5	7.8	7.1	7.4
		PchemNylon-6,6	6.5	0.0	6.5	8.8	8.0	8.4

[1)] The original process data used refer to the use of potato slurry proteins and potato steam peals (i.e., not for maize starch). Per tonne of hydrogen, around 2 tonnes of potato slurry proteins are required. It depends on the allocation approach how much land this translates to (we did not conduct calculations for land use).

[2)] This process uses fatty acids (FA) as feedstock for PDO, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane). In our calculations we exclusively assumed rapeseed oil with the typical production characteristics in Europe and assuming a price of rapeseed crude oil of 500 EURO/t.

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[*)] Negative emissions = carbon storage

[**)] Product value =Prod. cost + 30% capital charge

Table A10-4b): GHG emissions for bio-based and equivalent petrochemical-based platform chemicals and products – Sugar from SUGAR CANE

			GHG emissions			GHG emissions on a cradle-to-grave basis for three different end-of-life scenarios		
		Production system	GHG emissions cradle-to-grave	Renew. C stored in product (CO2 eq.)	GHG emissions cradle-to-factory gate	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Sugar Cane	(t CO_2eq./t)	(t CO_2/t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)
Alcohols	Ethanol	BioEtOH-SRI-Td	-0.3	-1.9	-2.2	-0.3	-1.0	-0.7
		BioEtOH-SRI-Corn-Td [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		BioEtOH-Anaer-GA-Tdcont	-0.6	-1.9	-2.5	-0.6	-1.3	-1.0
		BioEtOH-Anaer-GA-Fd	-0.7	-1.9	-2.6	-0.7	-1.4	-1.1
		BioEtOH-Anaer-GA-Fpv	-0.8	-1.9	-2.8	-0.8	-1.6	-1.3
		BioEtOH-SRI-Stover-Fd [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemEtOH-1 [2)]	2.0	0.0	2.0	3.9	3.2	3.5
		PchemEtOH-2 [2)]	1.3	0.0	1.3	3.2	2.5	2.8
	PDO	BioPDO-Anaer-SRI-Tdcont	1.3	-1.7	-0.4	1.3	0.7	0.9
		BioPDO-Aer-SRI-Tdcont	1.2	-1.7	-0.5	1.2	0.6	0.9
		BioPDO-Aer-DP-Tu	0.2	-1.7	-1.6	0.2	-0.4	-0.2
		BioPDO-Aer-GA-Tevbat	0.7	-1.7	-1.0	0.7	0.1	0.4
		BioPDO-Aer-GA-Tevcont	0.0	-1.7	-1.7	0.0	-0.6	-0.3
		BioPDO-Aer-GA-FpvH2O	0.9	-1.7	-0.9	0.9	0.3	0.5
		BioPDO-Aer-GA-FpvPDO	-0.6	-1.7	-2.3	-0.6	-1.2	-0.9
		BioPDO-Anaer-Glyc-SRI-Tdcont [3)]	3.4	-1.7	1.7	3.4	2.9	3.1
		BioPDO-Anaer-Glyc-VDI-Tdbat [3)]	3.5	-1.7	1.8	3.5	2.9	3.2
		PchemPDO-Propyl-DP	3.6	0.0	3.6	5.4	4.8	5.0
		PchemPDO-EO-SRI	2.3	0.0	2.3	4.1	3.5	3.7
		PchemPDO-Acro-SRI	4.4	0.0	4.4	6.1	5.5	5.8
	ABE	BioABE-Anaer-GA-Tdcont	0.7	-2.4	-1.7	0.7	-0.2	0.2
		BioABE-Anaer-GA-Tgscont	0.2	-2.4	-2.1	0.2	-0.6	-0.3
		BioABE-Anaer-GA-Fdm	-0.6	-2.4	-3.0	-0.6	-1.5	-1.1
		BioABE-Anaer-GA-Fmd	-2.0	-2.4	-4.4	-2.0	-2.8	-2.5
		BioABE-Anaer-GA-Fpv	-1.9	-2.4	-4.3	-1.9	-2.8	-2.4
		BioABE-Anaer-GA-Fgs	-1.3	-2.4	-3.7	-1.3	-2.2	-1.8
		PchemButanol	1.9	0.0	1.9	4.3	3.4	3.8
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	6.2	-1.5	4.7	6.2	5.8	6.0
		BioAcet-Anaer-GA-Ted	3.8	-1.5	2.3	3.8	3.4	3.6
		BioAcet-Anaer-GA-FexTOPO	2.5	-1.5	1.0	2.5	2.1	2.3
		BioAcet-Anaer-GA-FexDIPE	2.9	-1.5	1.4	2.9	2.5	2.7
		BioAcet-Anaer-GA-FedexDIPE	1.1	-1.5	-0.4	1.1	0.7	0.9
		BioAcet-Anaer-GA-Fed	1.4	-1.5	-0.1	1.4	1.0	1.2
		PchemAceticAcid	1.8	0.0	1.8	3.3	2.9	3.1
	Acrylic acid	BioAcryl-Anaer-GA-Fex	0.7	-1.8	-1.1	0.7	0.2	0.4
		PchemAcrylicAcid	1.7	0.0	1.7	3.5	3.1	3.2
	Lactic acid	BioLA-SRI-TpH6cont	1.6	-1.5	0.2	1.6	1.3	1.4
		BioLA-SRI-FlowpH	1.3	-1.5	-0.2	1.3	0.9	1.1
		BioLA-NW-Tu	0.9	-1.5	-0.6	0.9	0.5	0.7
		BioLA-Sh-Fex	0.8	-1.5	-0.6	0.8	0.5	0.6
		BioLA-Sh-Fed	0.8	-1.5	-0.7	0.8	0.4	0.5
		BioLA-Anaer-GA-Fed	0.2	-1.5	-1.3	0.2	-0.2	0.0
		BioLA-NW-Fu	0.2	-1.5	-1.3	0.2	-0.2	0.0
	Succinic acid	BioSA-Anaer-GA-Tc	3.5	-1.5	2.1	3.5	3.2	3.4
		BioSA-Anaer-GA-Ted	1.3	-1.5	-0.2	1.3	0.9	1.1
		BioSA-Aer-SRI-Fed	1.8	-1.5	0.3	1.8	1.5	1.6
		BioSA-Anaer-GA-Fcrx	1.1	-1.5	-0.4	1.1	0.8	0.9
		BioSA-Anaer-GA-Fc	2.1	-1.5	0.6	2.1	1.8	1.9
		BioSA-Anaer-GA-Fed	0.9	-1.5	-0.6	0.9	0.6	0.7
		PchemMaleicAnhydride	5.0	0.0	5.0	6.8	6.5	6.6
		PchemSA-MalAnhydr	7.1	0.0	7.1	8.6	8.3	8.4
	Adipic acid	BioAdip-Aer-GA-Tc	5.6	-1.8	3.8	5.6	5.1	5.3
		BioAdip-Aer-GA-Fc	1.6	-1.8	-0.2	1.6	1.2	1.3
		BioAdip-Aer-GA-Fed	0.5	-1.8	-1.4	0.5	0.0	0.2
		PchemAdipicAcid	4.0	0.0	4.0	5.8	5.3	5.5
	Citric acid	BioCit-Aer-SRI-Tevc [4)]	4.3	-1.4	2.9	4.3	4.1	4.2
		BioCit-Aer-SRI-Tix	2.1	-1.4	0.7	2.1	1.9	2.0
		BioCit-Aer-GA-Tpc	1.3	-1.4	-0.1	1.3	1.0	1.1
		BioCit-Aer-GA-Fc	0.3	-1.4	-1.0	0.3	0.1	0.2

[1)] The original process data used cover all steps starting with the intake of corn (for BioEtOH-SRI-Corn-Td) and corn stover (for BioEtOH-SRI-Stover-Fd). For this reason results can only be presented for these two feedstock types (see tables for maize starch and lignocellulosics).

[2)] Dataset PchemEtOH-1 is based on SRI data while dataset PchemEtOH-2 originates from the project C-STREAMS (Patel et al, 1999).

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[4)] The original process data used refer to the use of cane molasses. For this reason results are only presented for sugar cane as feedstock type and *not* for maize starch and lignocellulosics. Per tonne of citric acid, 2.6-2.8 tonnes of cane molasses are required. It depends on the allocation approach how much land this translates to (no allocation has been performed here).

		Production system	GHG emissions			GHG emissions on a cradle-to-grave basis for three different end-of-life scenarios		
			GHG emissions cradle-to-grave	Renew. C stored in product (CO2 eq.)	GHG emissions cradle-to-factory gate	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Sugar Cane	(t CO_2eq./t)	(t CO_2/t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	0.0	-2.3	-2.3	0.0	-0.8	-0.4
		PchemCapro	5.3	0.0	5.3	7.6	6.8	7.1
	Lysine	BioLys-Aer-SRI-Tix	7.7	-1.8	5.9	7.7	7.0	7.3
		BioLys-Aer-SRI-Tsp	0.6	-1.8	-1.2	0.6	0.0	0.3
		BioLys-Aer-GA-Tix	3.9	-1.8	2.1	3.9	3.2	3.5
		BioLys-Aer-GA-Fad	3.7	-1.8	1.9	3.7	3.1	3.3
H_2	Hydrogen	BioH2-A&F-gs [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemH2						
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	2.2	-2.6	-0.4	2.2	1.3	1.7
		BioPHAmcl-A&F-FA-Oilex [2)]	7.6	-2.6	5.0	7.6	6.7	7.1
		BioPHA-GA-Toa	-1.2	-2.6	-3.7	-1.2	-2.0	-1.7
		BioPHA-GA-Th	2.8	-2.6	0.2	2.8	1.9	2.2
		BioPHA-GA-Tey	3.8	-2.6	1.2	3.8	2.9	3.3
		BioPHA-GA-Tex	2.7	-2.6	0.1	2.7	1.8	2.2
		BioPHA-GA-Texey	3.7	-2.6	1.1	3.7	2.9	3.2
		BioPHA-GA-OilTexey [2)]	9.5	-2.6	6.9	9.5	8.6	9.0
		BioPHBV-SRI-Tey-1	4.7	-2.0	2.6	4.7	4.1	4.3
		BioPHB-SRI-Tey-2	-0.1	-2.0	-2.2	-0.1	-0.7	-0.4
		BioPHA-GA-Fey-1	0.7	-2.6	-1.9	0.7	-0.2	0.2
		BioPHA-GA-Fey-2	-0.3	-2.6	-2.9	-0.3	-1.2	-0.8
		PchemHDPE	1.6	0.0	1.6	4.7	3.5	4.0
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	-0.9	-3.1	-4.1	-0.9	-2.1	-1.6
		BioEthylene-BioEtOH-Anae-GA-Fpv	-1.4	-3.1	-4.5	-1.4	-2.6	-2.1
		PchemEthylene	1.3	0.0	1.3	4.4	3.2	3.7
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	2.3	-1.1	1.2	3.1	2.5	2.7
		EL-Sh-pchemEtOH-bioLA-F2	2.0	-1.1	0.9	2.8	2.2	2.5
		BioEL-NW-bioEtOH-bioLA-T1	0.9	-1.9	-1.0	0.9	0.3	0.6
		BioEL-Sh-bioEtOH-bioLA-F1	1.2	-1.9	-0.7	1.2	0.6	0.8
		BioEL-NW-bioEtOH-bioLA-F2	0.4	-1.9	-1.4	0.4	-0.1	0.1
		BioEL-Sh-bioEtOH-bioLA-F3	1.5	-1.9	-0.3	1.5	1.0	1.2
		BioEL-Sh-bioEtOH-bioLA-F4	1.2	-1.9	-0.6	1.2	0.7	0.9
		PchemEthylAcetate	1.9	0.0	1.9	3.9	3.3	3.5
		PchemBenzene	1.5	0.0	1.5	4.9	3.9	4.3
		PchemEGBE	1.8	0.0	1.8	4.0	3.0	3.4
		PchemMEK	3.3	0.0	3.3	5.7	4.8	5.2
		PchemAcetone	1.9	0.0	1.9	4.2	3.4	3.7
	PLA	BioPLA-bioLA-SRI-TpH6cont	2.8	-1.8	1.0	2.8	2.4	2.6
		BioPLA-bioLA-SRI-FlowpH	2.4	-1.8	0.5	2.4	1.9	2.1
		BioPLA-bioLA-NW-Tu	1.8	-1.8	0.0	1.8	1.4	1.6
		BioPLA-bioLA-Sh-Fex	1.8	-1.8	-0.1	1.8	1.3	1.5
		BioPLA-bioLA-Sh-Fed	1.7	-1.8	-0.1	1.7	1.2	1.4
		BioPLA-bioLA-Anaer-GA-Fed	0.9	-1.8	-0.9	0.9	0.5	0.7
		BioPLA-bioLA-NW-Fu	1.2	-1.8	-0.7	1.2	0.7	0.9
		PchemPET Amorph	3.3	0.0	3.3	5.6	5.0	5.3
		PchemPS	2.6	0.0	2.6	6.0	5.0	5.4
		PchemPE LD	1.9	0.0	1.9	5.0	3.8	4.3
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	2.4	-0.6	1.8	4.1	3.6	3.8
		PTT-bioPDO-Anaer-SRI-Tdcont	2.4	-0.6	1.8	4.2	3.6	3.8
		PTT-bioPDO-Aer-DP-Tu	2.0	-0.6	1.4	3.7	3.2	3.4
		PTT-bioPDO-Aer-GA-Tevbat	2.2	-0.6	1.6	3.9	3.4	3.6
		PTT-bioPDO-Aer-GA-Tevcont	2.0	-0.6	1.3	3.7	3.1	3.3
		PTT-bioPDO-Aer-GA-FpvH2O	2.3	-0.6	1.6	4.0	3.4	3.7
		PTT-bioPDO-Aer-GA-FpvPDO	1.8	-0.6	1.1	3.5	2.9	3.1
		PTT-bioPDO-Anaer-Glyc-SRI-Tdcont [3)]	3.2	-0.6	2.6	4.9	4.4	4.6
		PTT-bioPDO-Anaer-Glyc-VDI-Tdbat [3)]	3.3	-0.6	2.6	5.0	4.4	4.6
		PTT-PchemPDO-Propyl-DP	3.3	0.0	3.3	5.7	5.1	5.3
		PTT-PchemPDO-EO-SRI	2.8	0.0	2.8	5.2	4.6	4.8
		PTT-PchemPDO-EO-Shell	4.1	0.0	4.1	4.1	3.5	3.8
		PTT-PchemPDO-Acro-SRI	3.6	0.0	3.6	5.9	5.3	5.6
		PchemPET Amorph	3.3	0.0	3.3	5.6	5.0	5.3
		PchemNylon-6	5.5	0.0	5.5	7.8	7.1	7.4
		PchemNylon-6,6	6.5	0.0	6.5	8.8	8.0	8.4

[1)] The original process data used refer to the use of potato slurry proteins and potato steam peals. These results are reported in the table for maize starch.

[2)] This process uses fatty acids (FA) as feedstock for PDO, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane). In our calculations we exclusively assumed rapeseed oil with the typical production characteristics in Europe and assuming a price of rapeseed crude oil of 500 EURO/t.

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[*)] Negative emissions = carbon storage

[**)] Product value =Prod. cost + 30% capital charge

Table A10-4c): GHG emissions for bio-based and equivalent petrochemical-based platform chemicals and products – Sugar from LIGNOCELLULOSE

		Production system	GHG emissions			GHG emissions on a cradle-to-grave basis for three different end-of-life scenarios		
			GHG emissions cradle-to-grave	Renew. C stored in product (CO2 eq.)	GHG emissions cradle-to-factory gate	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Lignocellulosics	(t CO_2eq./t)	(t CO_2/t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)
Alcohols	Ethanol	BioEtOH-SRI-Td	0.5	-1.9	-1.4	0.5	-0.2	0.1
		BioEtOH-SRI-Corn-Td [1]	n/a	n/a	n/a	n/a	n/a	n/a
		BioEtOH-Anaer-GA-Tdcont	0.2	-1.9	-1.7	0.2	-0.5	-0.2
		BioEtOH-Anaer-GA-Fd	0.1	-1.9	-1.8	0.1	-0.6	-0.3
		BioEtOH-Anaer-GA-Fpv	0.0	-1.9	-1.9	0.0	-0.7	-0.4
		BioEtOH-SRI-Stover-Fd	1.5	-1.9	-0.4	1.5	0.8	1.1
		PchemEtOH-1 [2]	2.0	0.0	2.0	3.9	3.2	3.5
		PchemEtOH-2 [2]	1.3	0.0	1.3	3.2	2.5	2.8
	PDO	BioPDO-Anaer-SRI-Tdcont	2.1	-1.7	0.4	2.1	1.5	1.7
		BioPDO-Aer-SRI-Tdcont	1.9	-1.7	0.2	1.9	1.3	1.5
		BioPDO-Aer-DP-Tu	1.0	-1.7	-0.7	1.0	0.4	0.7
		BioPDO-Aer-GA-Tevbat	1.6	-1.7	-0.1	1.6	1.0	1.3
		BioPDO-Aer-GA-Tevcont	0.9	-1.7	-0.8	0.9	0.3	0.6
		BioPDO-Aer-GA-FpvH2O	1.6	-1.7	-0.2	1.6	1.0	1.2
		BioPDO-Aer-GA-FpvPDO	0.1	-1.7	-1.6	0.1	-0.5	-0.2
		BioPDO-Anaer-Glyc-SRI-Tdcont [3]	3.4	-1.7	1.7	3.4	2.9	3.1
		BioPDO-Anaer-Glyc-VDI-Tdbat [3]	3.5	-1.7	1.8	3.5	2.9	3.2
		PchemPDO-Propyl-DP	3.6	0.0	3.6	5.4	4.8	5.0
		PchemPDO-EO-SRI	2.3	0.0	2.3	4.1	3.5	3.7
		PchemPDO-Acro-SRI	4.4	0.0	4.4	6.1	5.5	5.8
	ABE	BioABE-Anaer-GA-Tdcont	1.8	-2.4	-0.5	1.8	1.0	1.3
		BioABE-Anaer-GA-Tgscont	1.4	-2.4	-1.0	1.4	0.5	0.9
		BioABE-Anaer-GA-Fdm	0.3	-2.4	-2.0	0.3	-0.5	-0.2
		BioABE-Anaer-GA-Fmd	-1.0	-2.4	-3.4	-1.0	-1.9	-1.5
		BioABE-Anaer-GA-Fpv	-1.0	-2.4	-3.3	-1.0	-1.8	-1.5
		BioABE-Anaer-GA-Fgs	-0.4	-2.4	-2.8	-0.4	-1.2	-0.9
		PchemButanol	1.9	0.0	1.9	4.3	3.4	3.8
Carboxylic acids	Acetic acid	BioAcet-Anaer-GA-TexTOPO	7.0	-1.5	5.5	7.0	6.6	6.7
		BioAcet-Anaer-GA-Ted	4.6	-1.5	3.1	4.6	4.2	4.4
		BioAcet-Anaer-GA-FexTOPO	2.9	-1.5	1.5	2.9	2.5	2.7
		BioAcet-Anaer-GA-FexDIPE	3.3	-1.5	1.8	3.3	2.9	3.1
		BioAcet-Anaer-GA-FedexDIPE	1.5	-1.5	0.0	1.5	1.1	1.3
		BioAcet-Anaer-GA-Fed	1.8	-1.5	0.3	1.8	1.4	1.6
		PchemAceticAcid	1.8	0.0	1.8	3.3	2.9	3.1
	Acrylic acid	BioAcryl-Anaer-GA-Fex	1.2	-1.8	-0.6	1.2	0.8	1.0
		PchemAcrylicAcid	1.7	0.0	1.7	3.5	3.1	3.2
	Lactic acid	BioLA-SRI-TpH6cont	2.1	-1.5	0.6	2.1	1.7	1.9
		BioLA-SRI-FlowpH	1.7	-1.5	0.3	1.7	1.3	1.5
		BioLA-NW-Tu	1.3	-1.5	-0.1	1.3	1.0	1.1
		BioLA-Sh-Fex	1.3	-1.5	-0.2	1.3	0.9	1.0
		BioLA-Sh-Fed	1.2	-1.5	-0.3	1.2	0.8	1.0
		BioLA-Anaer-GA-Fed	0.6	-1.5	-0.9	0.6	0.2	0.4
		BioLA-NW-Fu	0.6	-1.5	-0.9	0.6	0.2	0.4
	Succinic acid	BioSA-Anaer-GA-Tc	4.0	-1.5	2.5	4.0	3.7	3.8
		BioSA-Anaer-GA-Ted	1.7	-1.5	0.2	1.7	1.4	1.5
		BioSA-Aer-SRI-Fed	2.2	-1.5	0.7	2.2	1.9	2.0
		BioSA-Anaer-GA-Fcrx	1.5	-1.5	0.0	1.5	1.2	1.3
		BioSA-Anaer-GA-Fc	2.4	-1.5	0.9	2.4	2.1	2.3
		BioSA-Anaer-GA-Fed	1.2	-1.5	-0.2	1.2	0.9	1.1
		PchemMaleicAnhydride	5.0	0.0	5.0	6.8	6.5	6.6
		PchemSA-MalAnhydr	7.1	0.0	7.1	8.6	8.3	8.4
	Adipic acid	BioAdip-Aer-GA-Tc	7.8	-1.8	6.0	7.8	7.3	7.5
		BioAdip-Aer-GA-Fc	2.4	-1.8	0.6	2.4	2.0	2.2
		BioAdip-Aer-GA-Fed	1.3	-1.8	-0.5	1.3	0.8	1.0
		PchemAdipicAcid	4.0	0.0	4.0	5.8	5.3	5.5
	Citric acid	BioCit-Aer-SRI-Tevc [4]	4.3	-1.4	2.9	4.3	4.1	4.2
		BioCit-Aer-SRI-Tix	3.1	-1.4	1.7	3.1	2.8	2.9
		BioCit-Aer-GA-Tpc	2.6	-1.4	1.2	2.6	2.4	2.5
		BioCit-Aer-GA-Fc	0.7	-1.4	-0.6	0.7	0.5	0.6

[1] The original process data used cover all steps starting with the intake of corn. The results are therefore given in the table for starch maize starch.

[2] Dataset PchemEtOH-1 is based on SRI data while dataset PchemEtOH-2 originates from the project C-STREAMS (Patel et al, 1999).

[3] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[4] The original process data used refer to the use of cane molasses. For this reason results are only presented for sugar cane as feedstock type and *not* for maize starch and lignocellulosics.

		Production system	GHG emissions			GHG emissions on a cradle-to-grave basis for three different end-of-life scenarios		
			GHG emissions cradle-to-grave	Renew. C stored in product (CO2 eq.)	GHG emissions cradle-to-factory gate	Incineration without energy recovery	Incineration with energy recovery	Digestion with energy recovery
		Lignocellulosics	(t CO_2eq./t)	(t CO_2/t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)	(t CO_2eq./t)
N-compounds	Caprolactam	BioCapro-Aer-GA-Fd	1.0	-2.3	-1.4	1.0	0.2	0.5
		PchemCapro	5.3	0.0	5.3	7.6	6.8	7.1
	Lysine	BioLys-Aer-SRI-Tix	8.7	-1.8	6.9	8.7	8.1	8.4
		BioLys-Aer-SRI-Tsp	1.9	-1.8	0.1	1.9	1.2	1.5
		BioLys-Aer-GA-Tix	5.6	-1.8	3.8	5.6	4.9	5.2
		BioLys-Aer-GA-Fad	4.9	-1.8	3.1	4.9	4.3	4.5
H_2	Hydrogen	BioH2-A&F-gs [1)]	n/a	n/a	n/a	n/a	n/a	n/a
		PchemH2						
Polymer	PHA	BioPHAmcl-A&F-D5:FA1-Tex	3.2	-2.6	0.6	3.2	2.3	2.6
		BioPHAmcl-A&F-FA-Oilex [2)]	7.6	-2.6	5.0	7.6	6.7	7.1
		BioPHA-GA-Toa	0.1	-2.6	-2.5	0.1	-0.8	-0.4
		BioPHA-GA-Th	3.9	-2.6	1.4	3.9	3.1	3.4
		BioPHA-GA-Tey	5.0	-2.6	2.4	5.0	4.1	4.5
		BioPHA-GA-Tex	3.8	-2.6	1.3	3.8	3.0	3.3
		BioPHA-GA-Texey	4.9	-2.6	2.3	4.9	4.0	4.4
		BioPHA-GA-OilTexey [2)]	9.5	-2.6	6.9	9.5	8.6	9.0
		BioPHBV-SRI-Tey-1	5.8	-2.0	3.8	5.8	5.2	5.5
		BioPHB-SRI-Tey-2	1.0	-2.0	-1.0	1.0	0.5	0.7
		BioPHA-GA-Fey-1	1.6	-2.6	-1.0	1.6	0.7	1.1
		BioPHA-GA-Fey-2	0.6	-2.6	-2.0	0.6	-0.3	0.1
		PchemHDPE	1.6	0.0	1.6	4.7	3.5	4.0
Products derived from WB chemicals	Ethylene	BioEthylene-BioEtOH-Anaer-GA-Td	0.5	-3.1	-2.7	0.5	-0.7	-0.2
		BioEthylene-BioEtOH-Anae-GA-Fpv	0.0	-3.1	-3.2	0.0	-1.2	-0.7
		PchemEthylene	1.3	0.0	1.3	4.4	3.2	3.7
	Ethyl lactate	EL-Sh-pchemEtOH-bioLA-F1	2.6	-1.1	1.5	3.4	2.8	3.1
		EL-Sh-pchemEtOH-bioLA-F2	2.4	-1.1	1.2	3.1	2.5	2.8
		BioEL-NW-bioEtOH-bioLA-T1	1.6	-1.9	-0.3	1.6	1.0	1.2
		BioEL-Sh-bioEtOH-bioLA-F3	1.8	-1.9	0.0	1.8	1.3	1.5
		BioEL-Sh-bioEtOH-bioLA-F4	1.9	-1.9	0.0	1.9	1.3	1.6
		PchemEthylAcetate	1.9	0.0	1.9	3.9	3.3	3.5
		PchemBenzene	1.5	0.0	1.5	4.9	3.9	4.3
		PchemEGBE	1.8	0.0	1.8	4.0	3.0	3.4
		PchemMEK	3.3	0.0	3.3	5.7	4.8	5.2
		PchemAcetone	1.9	0.0	1.9	4.2	3.4	3.7
	PLA	BioPLA-bioLA-SRI-TpH6cont	3.4	-1.8	1.5	3.4	2.9	3.1
		BioPLA-bioLA-SRI-FlowpH	2.9	-1.8	1.1	2.9	2.5	2.7
		BioPLA-bioLA-NW-Tu	2.4	-1.8	0.6	2.4	2.0	2.2
		BioPLA-bioLA-Sh-Fex	2.3	-1.8	0.5	2.3	1.9	2.1
		BioPLA-bioLA-Sh-Fed	2.2	-1.8	0.4	2.2	1.8	2.0
		BioPLA-bioLA-Anaer-GA-Fed	1.4	-1.8	-0.4	1.4	1.0	1.2
		BioPLA-bioLA-NW-Fu	1.7	-1.8	-0.1	1.7	1.3	1.5
		PchemPET Amorph	3.3	0.0	3.3	5.6	5.0	5.3
		PchemPS	2.6	0.0	2.6	6.0	5.0	5.4
		PchemPE LD	1.9	0.0	1.9	5.0	3.8	4.3
	PTT	PTT-bioPDO-Aer-SRI-Tdcont	2.7	-0.6	2.0	4.4	3.8	4.0
		PTT-bioPDO-Anaer-SRI-Tdcont	2.7	-0.6	2.1	4.4	3.9	4.1
		PTT-bioPDO-Aer-DP-Tu	2.3	-0.6	1.7	4.0	3.5	3.7
		PTT-bioPDO-Aer-GA-Tevbat	2.6	-0.6	1.9	4.3	3.7	3.9
		PTT-bioPDO-Aer-GA-Tevcont	2.3	-0.6	1.7	4.0	3.4	3.7
		PTT-bioPDO-Aer-GA-FpvH2O	2.6	-0.6	1.9	4.3	3.7	3.9
		PTT-bioPDO-Aer-GA-FpvPDO	2.0	-0.6	1.4	3.7	3.1	3.4
		PTT-bioPDO-Anaer-Glyc-SRI-Tdcont [3)]	3.2	-0.6	2.6	4.9	4.4	4.6
		PTT-bioPDO-Anaer-Glyc-VDI-Tdbat [3)]	3.3	-0.6	2.6	5.0	4.4	4.6
		PTT-PchemPDO-Propyl-DP	3.3	0.0	3.3	5.7	5.1	5.3
		PTT-PchemPDO-EO-SRI	2.8	0.0	2.8	5.2	4.6	4.8
		PTT-PchemPDO-EO-Shell	4.1	0.0	4.1	4.1	3.5	3.8
		PTT-PchemPDO-Acro-SRI	3.6	0.0	3.6	5.9	5.3	5.6
		PchemPET Amorph	3.3	0.0	3.3	5.6	5.0	5.3
		PchemNylon-6	5.5	0.0	5.5	7.8	7.1	7.4
		PchemNylon-6,6	6.5	0.0	6.5	8.8	8.0	8.4

[1)] The original process data used refer to the use of potato slurry proteins and potato steam peals. These results are reported in the table for maize starch. It depends on the allocation approach how much land this translates to (we did not conduct calculations for land use).

[2)] This process uses fatty acids (FA) as feedstock for PDO, e.g. tall oil fatty acids (TOFA), coconut oil fatty acids (COFA), linseed oil or rapeseed oil (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane). In our calculations we exclusively assumed rapeseed oil with the typical production characteristics in Europe and assuming a price of rapeseed crude oil of 500 EURO/t.

[3)] The data in this row refer to the fermentation of glycerol (i.e., not to fermentable sugar from maize starch, lignocellulosics or sugar cane).

[*)] Negative emissions = carbon storage

[**)] Product value =Prod. cost + 30% capital charge

Appendix 11: Scenario assumptions

A11-1: Prices of fossil fuels and related inputs for chemical production

	Gas			Coal			Oil		
	2000	2020	2050	2000	2020	2050	2000	2020	2050
A1-ASF	1	1	1.06	1	1.07	1.27	1	1.2	1.61
A1-Minicam	1	1.17	1.58	1	1.14	1.36	1	1.22	1.48
GE-CPB	1	1.08	1.28	-	-	-	1	1.07	1.32
A1B-Message	1	1.72	2.14	1	1.32	1.05	1	1.79	1.53
A1G-Message	1	1.15	2.55	1	1.1	1.5	1	1.48	2.33
A1T-Message	1	1.12	1.65	1	1.03	1.29	1	1.41	1.7
A1C-Message	1	1.16	2.16	1	1.46	1.88	1	1.47	1.93
B1-ASF	1	0.98	0.96	1	1.07	1.13	1	1.16	1.43
B1-Minicam	1	1.07	1.34	1	1.14	1.21	1	1.13	0.97
SE-CPB	1	1.04	1	-	-	-	1	1.05	0.93
B1G-Message	1	1.33	1.61	1	1.59	1.15	1	1.83	2.14
B1-Message	1	1.22	1.3	1	1.49	0.97	1	1.66	1.21
B1T-Message	1	1.26	0.94	1	1.31	0.94	1	1.62	1.15
A2-ASF	1	1	1	1	1	1.13	1	1.07	1.41
A2-Minicam	1	1.2	2.14	1	1.16	1.36	1	1.26	1.64
TM-CPB	1	1.19	1.24	-	-	-	1	1.14	1.32
A2-Message	1	1.38	2.4	1	1.01	1.54	1	1.88	3.31
B2-ASF	1	1	0.98	1	1	1.07	1	1.07	1.39
B2-Minicam	1	1.13	1.41	1	1.14	1.21	1	1.11	1.09
RC-CPB	1	1	0.9	-	-	-	1	1.05	1.11
B2-Message	1	1.19	1.8	1	1.76	1.38	1	1.51	2.64

The CPB model used the SRES scenarios as basis for comparable scenarios used for modeling the European economy. The other models are included in the special report of the IPCC on emission scenarios.

Table A11-1: Development of fossil fuel prices in different models using the SRES scenario (IPCC SRES, CPB, Personal communication IASA)

A11-2: Electricity price calculation

Electricity prices in the different scenarios are calculated as power generation cost including fixed capital depreciation, averaged across the energy mix (gas, coal, oil, nuclear, biomass and hydropower) in the EU in the year 2000. Techno-economic data for power generation e.g. investment costs, energy conversion efficiency etc. are taken from Smekens et al. (2003). A 10% discount rate over a depreciation period of 15 years[120] has been assumed, corresponding to a 13.5% annual capital charge. Table A11-3 presents an overview of the adopted parameters[121] and Table A11-4 shows the resulting electricity costs for the different scenarios.

[120] Parameters reported by Framatome at the UNECE Roundtable Facilitating Investment in the Electricity Sector in the Transition Economies, Geneva, 19. Nov. 2003. http://www.unece.org/ie/se/pp/elec/framatome.pdf

[121] For consistency with BREW's standard utility prices and since data on variable costs for nuclear power generation are missing, this parameter is to adjust electricity prices to the base price of 5.45 Eurocent/kWh.

Energy carrier	Share of power production %	Electric efficiency %	Investment costs €/kW	Fixed costs $/kW	Workload h/yr	Capital charge %
Gas	6.21	55	510	10	7000	13.5
Coal	39.7	38	1125	35	7000	13.5
Oil	6.47	45	825	20	7000	13.5
Nuclear	30.4	35	1710	57.5	7000	13.5
Biomass	1.32	38	1600	43	7000	13.5
Other Renewables	15.9	1	1850	30	4500	13.5

Table A11-2a: Techno-economic characteristics of electricity production in Europe

Scenario	LOW	MEDIUM	HIGH
2000	5.45	5.45	5.45
2010	5.52	5.64	5.70
2020	5.53	5.77	5.90
2030	5.55	5.91	6.11
2040	5.56	6.05	6.31
2050	5.58	6.19	6.51

Table A11-2b: Electricity prices in (Eurocent/kWh) in the different scenarios

A11-3: Prices of intermediates

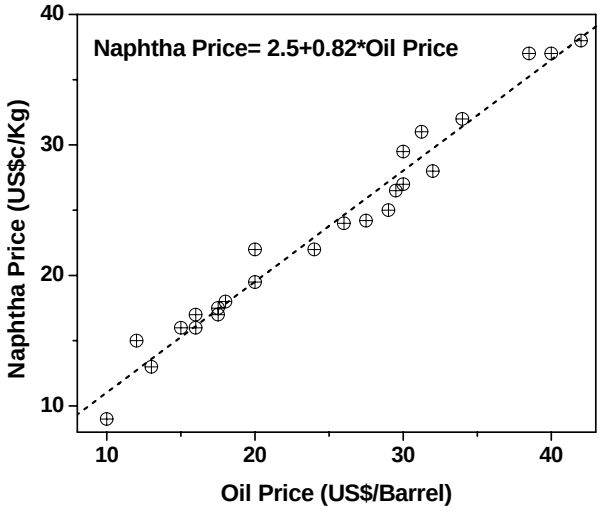
Raw material	SRI process	Share of feedstock on production value	Share of utilities on production value
Acetaldehyde	Acetaldehyde from ethyelene by one-step oxidation	Ethylene 59.3%	Electricity 3.9%, Steam 0.4%
Acetone	No specific process data for typical production from Cumene	Ratio taken from benzene	
Ammonia	Ammonia from natural gas by steam reforming (ICI AMV process)	Natural gas (also fuel): 29.8%	Electricity 1.3%
Benzene	Benzene and Toluene from refromate by Carom ™ Extraction	Crude oil derivatives 58.7%	Natural gas 2.2%; Steam 1.8%
n-Butane	No specific process available in SRI data	Ratio taken from crude oil	
BTX	BTX production from LPG	Crude oil derivatives 39.8%	Steam 4.4%; Electricity 2.3%; Natural gas 2.3%
Cyclohexane	Cyclohexane from Benzene by hydrogenation	Hydrogen 19.6%; Benzene 63.4%	
Diethylene glycol	No specific process available in SRI data	Ratio taken from ethylene glycol	
Ethylbenzene	Ethylbenzene from benzene by liquid-phase Alkylation, AlCl3 CAT.	Ethylene 35.3%; Benzene 54.6%	
Formaldehyde	Formaldehyde from Methanol, Ferric-Molybdata catalyst	Methanol 33.0%	Electricity –1.6%; Steam 0.8%
Hydrogen	Hydrogen from natural gas by steam reforming	Natural gas 41.9%	Electricity 0.7%; Steam –3.1%
Hydroquinone	Hydroquinone from propylene and benzene via P-Diisopropyl benzene	Propylene 7.9%; Benzene 5.2%;	Steam 1.8%; Electricity 0.3%; Fuel oil 2.2%
Isobutanol	No specific process available in SRI data	Ratio taken from propylene	
Methanol	Methanol from natural gas by the ICI LCM process	Natural gas 47.2%	
Methyl acetate	No specific process available in SRI data	Ratio taken from methanol	
Naphtha	No specific process available in SRI data	Fitting of historical data	
Octanoic acid	No specific process available in SRI data	Ratio taken from crude oil	
Toluene	No specific process available in SRI data	Ratio taken from BTX	

Data SRI (2000). Used are data for medium scale production units at 100% load.

Table A11-3: Variation of raw material costs depending on fossil feedstock and utilities

A11-4: Approximating naphtha prices

Naphtha is one of the main refinery commodities that is produced mainly by atmospheric distillation. Profit margins are limited and the price of crude oil. Figure A11-1 shows the relationship between naphtha prices and crude oil prices (Brent) from 1992 to 2001. The correlation is used to determine naphtha prices as a function of different crude oil prices in the scenarios.



(Data Source: http://www.platts.com/)

Figure A11-1: Correlation between crude oil price and naphtha price

A11-5: Future demand of chemicals

Annual growth	CleanTech Base	CleanTech High	CleanTech Low	VLEEM Base	CPB GE	CPB TM	CPB SE	CPB RC
	Plastics	Plastics	Plastics	Plastics	Total chemicals	Total chemicals	Total chemicals	Total chemicals
1999-2010	2.5 %	3.5 %	1.5 %	1.5 %	5.1 %	3.5 %	3.0 %	1.9 %
2010-2020	2.0 %	3.0 %	1.0 %	2.3 %	5.1 %	3.5 %	3.0 %	1.9 %
2020-2030	1.5 %	2.0 %	0.5 %	1.9 %	5.1 %	3.5 %	3.0 %	1.9 %
2030-2040	-	-	-	1.6 %	5.1 %	3.5 %	3.0 %	1.9 %
2040-2050	-	-	-	1.4 %	5.1 %	3.5 %	3.0 %	1.9 %

Data source: CleanTech – Phylipsen et al., 2004; VLEEM- Chateau et al., 2005; CPB – Lejour, 2003.

Table A11-5a: Projected annual growth of the physical production of chemicals in Europe

Scenario	Base	LOW					MEDIUM					HIGH				
	2000	2010	2020	2030	2040	2050	2010	2020	2030	2040	2050	2010	2020	2030	2040	2050
PE	11300	11300	11300	11300	11300	11300	13114	15219	17663	20498	23789	15186	20409	27428	36861	49538
PTT	524	524	524	524	524	524	608	706	819	951	1103	704	946	1272	1709	2297
Nylon 6	1255	1255	1255	1255	1255	1255	1456	1690	1962	2277	2642	1687	2267	3046	4094	5502
PET	3500	3500	3500	3500	3500	3500	4062	4714	5471	6349	7368	4704	6321	8495	11417	15344
PS	3365	3365	3365	3365	3365	3365	3905	4532	5260	6104	7084	4522	6078	8168	10977	14752
Ethyl lactate	310	310	310	310	310	310	360	418	485	562	653	417	560	752	1011	1359
Ethyl acetate	310	310	310	310	310	310	360	418	485	562	653	417	560	752	1011	1359
Ethylene *)	19402	19402	19402	19402	19402	19402	22517	26132	30327	35196	40846	26075	35042	47094	63290	85057
Maleic Anhydr.	380	380	380	380	380	380	441	512	594	689	800	511	686	922	1240	1666
Adipic acid	1000	1000	1000	1000	1000	1000	1161	1347	1563	1814	2105	1344	1806	2427	3262	4384
Acetic acid	1400	1400	1400	1400	1400	1400	1625	1886	2188	2540	2947	1881	2529	3398	4567	6137
n-Butanol	930	930	930	930	930	930	1079	1253	1454	1687	1958	1250	1680	2257	3034	4077
Total*	31004	31004	31004	31004	31004	31004	35982	41758	48462	56242	65271	41667	55997	75255	101137	135919

*) The value in the row “Total” is smaller than the total of the individual rows. The reason is that the entries in row “Total” are corrected for the use of ethylene for the production of polyethylene (PE), ethylacetate, polyethyleneterephthalate (PET) and polystyrene (PS).

Table A11-5b: Projected volumes of chemical production in Europe in the various scenarios in kton p.a.

Appendix 12: Calculation of economic potentials

A12-1: Processes for the calculation of product values

Bio-based chemical	State –of –the Art Technology	Future technology
Acetic acid	Acetic acid via anaerobic fermentation on dextrose substrate; workup via extraction using TOPO; Generic Approach (today); *BioAcet-Anaer-GA-Tex1*	Acetic acid via anaerobic fermentation on dextrose substrate; workup via evaporation+distillation; Generic Approach (future); *BioAcet-Anaer-GA-Fevd*
Adipic acid	Adipic acid via aerobic fermentation on glucose substrate; workup via evaporation, crystallisation; Generic Approach (today); *BioAdip-Aer-GA-Tc*	Adipic acid via aerobic fermentation on glucose substrate; workup via electrodialysis; Generic Approach (future); *BioAdip-Aer-GA-Fed*
n-Butanol	ABE via anaerobic fermentation on dextrose substrate; workup via distillation; Generic Approach (today); *ABE-Anaer-GA-Td*	ABE via anaerobic fermentation on dextrose substrate; workup via pervaporation; Generic Approach (future); *ABE-Anaer-GA-Fpv*
Ethyl lactate	Ethyl lactate via pervaporation-assisted esterification of lactic acid on dextrose substrate. One step process; low pH fermentation of lactic acid; lactic acid is not isolated. (Shell confidential data); *EL-Sh-pv*	No specific process data, price, energy and GHG emission depreciation as for PLA assumed
Ethylene	Dehydration of Bio-ethanol (Shell confidential data); Bio-ethanol via anaerobic continuous fermentation on dextrose substrate; workup via distillation; Generic Approach (present); *BioEtOH-Anaer-GA-Tdcont*	Dehydration of Ethanol (Shell confidential data); Bio-ethanol via anaerobic fermentation on dextrose substrate; workup via pervaporation; Generic Approach (future); *BioEtOH-Anaer-GA-Fpv*
PHA	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; Generic Approach (present); *PHA–GA-Toa*	Mid chain length poly(hydroxyalkanoate) in latex form via fermentation on dextrose; Generic Approach (present); *PHA–GA-Toa (future worse than today case)*
PLA	Poly(lactic acid) via polycondensation of lactic acid (NatureWorks). lactic acid via fermentation by xxx on dextrose; workup via unspecified process involving neutralisation & acidification. NatureWorks process; supplementary data from SRI process designs; *PLA-LA-NW-Tu*	Poly(lactic acid) via polycondensation of lactic acid (NatureWorks). Lactic acid via fermentation on dextrose; workup via electrodialysis. Generic approach, future case; *PLA-LA-NW-Fu*
PTT	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid, Bio-1,3-PDO via aerobic cont. bioprocess on dextrose substrate, workup by evaporation and distillation; Generic Approach today; *BioPTT-Aer-GA-Tevcont*.	Poly(trimethylene terephthalate) via polycondensation of bio-1,3-propanediol and purified terephthalic acid, Bio-1,3-PDO via aerobic cont. bioprocess on dextrose substrate, workup by pervaporation of PDO, Generic Approach future; *BioPDO-Aer-GA-FpvPDO*
Succinic acid	Bio-succinic acid via fermentation by Actinobacillus succinogenes 130Z on dextrose substrate; workup via electrodialysis; Generic Approach, today. *BioSA-GA-Ted*	Bio-succinic acid via fermentation by Actinobacillus succinogenes 130Z on dextrose substrate; workup via crystallisation and redox; Generic Approach, future; *BioSA-GA-Fcrx*

Table A12-1a: Processes for the production of bio-based chemicals (compare also Appendix A7)

Petrochemical	Process
Acetic acid	From MEOH by low pressure carbonylation, supported Rh Catalyst
Adipic acid	From cyclohexane
n-Butanol	From propylene, cobalt phosphine catalyst
Ethyl acetate	Ethyl acetate via pervaporation-assisted esterification of acetic acid
Ethylene	From wide-range naphtha steamcracking
HDPE	By liquid phase slurry process
PET	From DMT and EG
PS	General purpose PS, continous bulk polymerization
PTT	Via polycondensation of 1,3-propanediol (from Ethylene oxide) and purified terephthalic acid
Nylon 6	From Caprolactam
Maleic Anhydride	From n-butane, moving bed reactor

Table A12-1b: Processes for the production of reference petrochemicals (data from SRI 2000)

A12-2: Economic potentials

Characteristic	Share of bio-based chemicals of total technical potential	Product value ratio (Petrochemical/bio-based)
Green premium	30%	0.5
Without green premium	5%	0.9
Easy implementation	95%	1.0
Easy implementation full potential	100%	1.1
Difficult implementation	80%	1.1
Difficult implementation full potential	100%	1.3

Table A12-2: Economic substitution potentials (see Figure 4-3)

Appendix 13: Result: Market potentials of bio-based chemicals

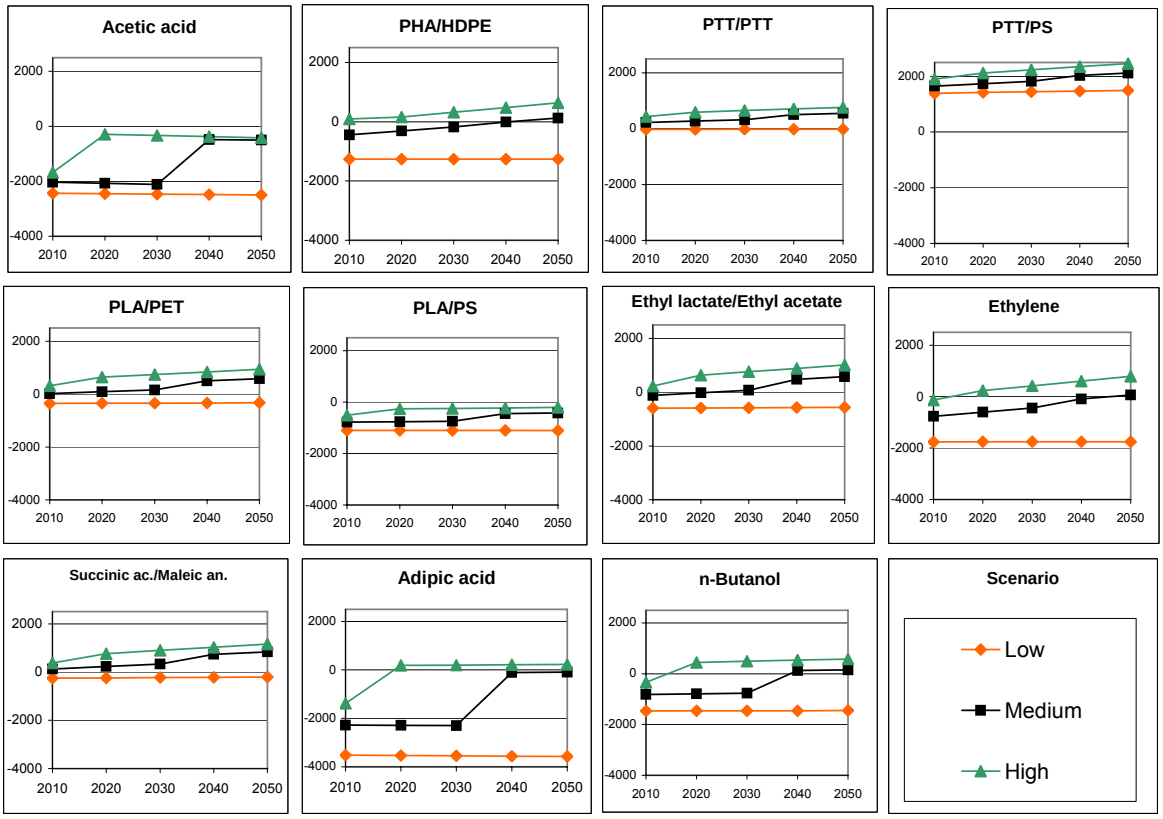


Figure A13-1: Differences between the product values of the reference petrochemical and the bio-based chemical in €/t (positive values show an advantage of the bio-based chemical)

	Feedstock	Scenario	2010	2020	2030	2040	2050
Energy savings in %	starch	LOW	0.0%	4.2%	6.6%	7.1%	7.1%
	lignocellulose	LOW	0.0%	5.6%	9.4%	10.3%	10.3%
	starch	MEDIUM	3.7%	8.6%	10.4%	15.0%	20.4%
	lignocellulose	MEDIUM	6.3%	13.1%	16.0%	20.4%	30.5%
	starch	HIGH	6.3%	23.2%	31.6%	38.5%	38.7%
	lignocellulose	HIGH	10.7%	36.7%	52.4%	66.5%	66.7%
GHG emission Reduction in %	starch	LOW	0.0%	4.1%	6.9%	7.5%	7.6%
	lignocellulose	LOW	0.0%	5.2%	9.2%	10.1%	10.1%
	starch	MEDIUM	4.1%	9.3%	11.5%	15.8%	21.5%
	lignocellulose	MEDIUM	6.2%	12.8%	16.0%	20.2%	29.6%
	starch	HIGH	7.2%	24.5%	33.5%	41.0%	41.1%
	lignocellulose	HIGH	10.7%	35.4%	50.1%	63.4%	63.6%

Table A13-1: Energy savings and GHG emission reduction by bio-based chemical production compared to the production of all chemicals from fossil fuel in the three scenarios

Comparison	**PHA/ HDPE**	**PTT/ PTT**	**PTT/ Nylon 6**	**PLA/ PET**	**PLA/ PS**	**Ethylene/ Ethylene**	**Succ. a./ Mal. anh.**	**Adipic a./ adipic a.**	**Acetic a./ acetic a.**	**n-Butanol/ n-Butanol**
Petchem prod.value - bio product values	-442.8	224.1	1653.3	21.3	-776.1	-766.5	121.6	-2282.7	-2031.6	-810.0
Petchem market price - bio product value	-582.0	25.9	1733.1	-384.4	-514.4	-852.4	-236.8	-960.0	-2025.5	-404.6
Total difference between approaches	*-139.2*	*-198.2*	*79.7*	*-405.8*	*261.7*	*-85.9*	*-358.4*	*1322.7*	*6.2*	*405.4*

Table A13-2: Comparison of product values and current market prices of petrochemicals to bio-based chemical product values at the short term (i.e. 2010). Results refer to the MEDIUM scenario

For most products it is not important for their short-term market potential in the MEDIUM scenario, whether the petrochemicals are compared by means of product values or market prices to the bio-based chemicals. Just in the case of PLA, it replaces PET if compared to the product value but not if compared to the market price.

Appendix 14: Questionnaire of the BREW survey

Survey
Stakeholders' perceptions of the biotechnological production of bulk chemicals from renewable resources

Please send back the filled in questionnaire ***by December 3, 2004*** to

Fabio Terragni
North Milan Development Agency (ASNM)
Via Venezia 23
20099 Sesto San Giovanni (Mi)
Italy

Fax +39 02 24126 541, E-mail: WhiteBiotech@isi.fraunhofer.de

Part 1

1.	Person filling in this questionnaire
Name	
Position, Function	
E-Mail	
Fax	
Name and Postal Address of Company/Institution/Organisation	
Internet-Homepage	http://

2.	I wish to receive the results of this survey	Yes ❑	No ❑

3.	The survey topic is NOT at all relevant for my company/institution/organisation *If you have ticked this box, please send back the questionnaire. Otherwise proceed with the following questions.*	❑

In order to guarantee your privacy and anonymity, this part of the questionnaire will be separated from your following responses. We will not publish any results that would allow anyone to identify the answers you gave.

4.	My company/institution/organisation is an institution of the following type (tick only one box):		
Research institute, university	❑	Company	❑
Policy, governmental organisation	❑	Non-governmental organisation (NGO), industrial association	❑
Other, please specify:	❑	_____	

5.	I am/my company/institution/organisation is active in the following field (tick only one box):		
Agriculture, renewable resources, plant breeding	❑	Chemical industry	❑
Industrial sector downstream of the chemical industry	❑	Biotechnology	❑
Environment	❑	Energy	❑
Consumers	❑	Others, please specify: _____	❑

6.	The biotechnological production of chemicals from biomass is being dealt with in my company/institution/organisation in the following way:				
We are active in this field	❑	Not yet active, but may enter the field or deal with the issue in the future	❑	Not active, neither today nor in the future	❑

7.	My knowledge and overview of biotechnological production of chemicals from biomass can be characterised in the following way:				
I am an expert in this field	❑	I am quite well informed and knowledgeable	❑	I have never or only occasionally heard/read about it	❑

Part 2: Putting the biotechnological production of bulk chemicals into perspective

The biotechnological production of bulk chemicals from biomass competes with the conventional production of chemicals from fossil fuels. Moreover, biomass could alternatively be used as food or feed, or for bioenergy production. In this part of the questionnaire, we ask you to put biotechnological bulk chemicals production into perspective with these competing options. In answering the following questions, please assume

- that the biotechnological production of bulk chemicals occurs in Europe and that it is performed at substantial scale,

- that additional requirements for the biotechnological production of bulk chemicals will NOT lead to land scarcity for food and other uses (e.g. feed, bioenergy) in Europe or elsewhere.

8.	What is your opinion of the following concepts to achieve the long-term goal of sustain-ability? Please tick the appropriate box.

Concept	Is sustainable	Can become sustainable if improved	Is not sustainable
Food/feed production by conventional agriculture	❑	❑	❑
Food/feed production by organic agriculture	❑	❑	❑
Energy production from fossil fuels	❑	❑	❑
Energy production from renewable resources	❑	❑	❑
Energy production from biomass	❑	❑	❑
Bulk chemicals derived from fossil resources by chemical synthesis	❑	❑	❑
Bulk chemicals derived from biomass by biotechnology	❑	❑	❑

9.	In your opinion, how important are the following concepts in the coming 30 years to achieve the long-term goal of sustainability?

Concept	Is of major importance	Is of medium importance	Is of minor importance
Shift from conventional to organic agriculture	❑	❑	❑
Shift from conventional to renewable energy production	❑	❑	❑
Shift from chemical bulk chemicals production from fossil resources to biotechnological bulk chemicals production from biomass	❑	❑	❑

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10.	Bulk chemicals can be obtained from biomass or fossil fuels. Which of these two options is preferable in your view?		
a) nowadays		For which reasons?	
Chemicals from biomass	❑	Environmental reasons	❑
Chemicals from fossil fuels	❑	Economic reasons	❑
Both	❑	Geo-political reasons	❑
None	❑	Technical feasibility	❑
Don't know	❑	Other; please specify: _____	❑
b) in the future		For which reasons?	
Chemicals from biomass	❑	Environmental reasons	❑
Chemicals from fossil fuels	❑	Economic reasons	❑
Both	❑	Geo-political reasons	❑
None	❑	Technical feasibility	❑
Don't know	❑	Other; please specify: _____	❑

11.	Biomass can be used for producing either chemicals or energy. Which of these two options is preferable in your view?		
a) nowadays		For which reasons?	
Chemicals from biomass	❑	Environmental reasons	❑
Energy from biomass	❑	Economic reasons	❑
Both	❑	Geo-political reasons	❑
None	❑	Technical feasibility	❑
Don't know	❑	Other; please specify: _____	❑
b) in the future		For which reasons?	
Chemicals from biomass	❑	Environmental reasons	❑
Energy from biomass	❑	Economic reasons	❑
Both	❑	Geo-political reasons	❑
None	❑	Technical feasibility	❑
Don't know	❑	Other; please specify: _____	❑

12.	Should European governments support European industry with the goal to attain a leading role on global markets in the biotechnological production of chemicals from biomass even if the production were to take place to a large extent outside Europe (e.g. in Latin America and Africa)?	
Yes ❑	No ❑	Don't know ❑

13.	There are several environmental and health risks inherent in the use of biotechnology for the manufacturing of chemicals from biomass. All in all, do you think that these risks can be managed in such a way that they become acceptable and in balance with the benefits?	
Yes, sure ❑	Yes, I am confident that this can be achieved ❑	It depends ❑
I am sceptical that this can be achieved ❑	No, by no means ❑	Don't know ❑

14.	Will the biotechnological production of bulk chemicals from biomass become an important area for innovation and economic growth in the next 30 years?	
Yes ❑	No ❑	Don't know ❑

15.	Will the biotechnological production of bulk chemicals from biomass revitalise the petrochemical industry and contribute substantially to its international competitiveness in the next 30 years?	
Yes ❑	No ❑	Don't know ❑

Part 3: Exploring views of different technological options for bulk chemicals production in detail

This part of the questionnaire focuses on the biotechnological production of bulk chemicals from biomass. A plastic was chosen here as an example for a bulk chemical. Biotechnology offers different technological options for manufacturing a bulk chemical. These options differ in various aspects, making the choice of "the best" option complex and difficult. In the following part of the questionnaire, we would like to explore your reasoning in making this choice between competing options.

Please imagine that a new production process for a certain sort of plastic is to be established, with the goal to produce this plastic in 2030 in bulk quantities. A plastic with the desired properties could be made accessible via four different manufacturing routes: the classical chemical manufacturing route starting from fossil resources (Option A), and three biotechnological routes involving biomass (Options B-D):

Option A:

The chemical industry produces a plastic with the desired properties by chemical synthesis from fossil fuels and sells it to the plastic processing industry.

Option B:

The chemical industry produces a naturally occurring bioplastic (e.g. a bioplastic such as polyhydroxyalkanoate, PHA) which has the same properties as the plastic in option A. Bacteria, which naturally produce this bioplastic, are grown in a closed reactor. Sugars derived from an agricultural crop which is grown for this purpose (e.g. wheat or maize) are used as feedstock for this bacterial fermentation.

Option C:

Same as option B except that the production organism is genetically modified (genetically engineered by the application of gene technology) in order to optimize its production characteristics.

Option D:

Farmers grow special agricultural crop plants which synthetise the same bioplastic as in options B and C. The ability to synthesize the bioplastic in the crop has been conferred to these plants by genetic modification. The plants are delivered to the chemical industry which extracts the bioplastic and sells it to the plastic processing industry.

The three biotechnological routes have the following steps in common:

- The production organism is grown, the organism synthesizes the bioplastic during its growth and the bioplastic accumulates within the organism.
- After harvest of the production organisms, the bioplastic is extracted from the organisms and purified.
- The resulting bioplastic pellets can be shipped and converted to final products as conventional petrochemical plastics.
- The residual biomass can be used as animal feed, fertiliser in agriculture, or for energy production.

The specific features of each of these four options are summarised in the following table. Please familiarise yourself with these characteristics before proceeding to the assessment itself.

Key characteristic	Option A	Option B	Option C	Option D
Option short title	**Chemical production/fossil**	**Biotechnological production/biomass**		
	Chemical production	Bacteria	Genetically modified bacteria	Genetically modified plants
Product	Plastic with similar properties as the bioplastic	A naturally occuring bioplastic, such as PHA (polyhydroxyalkanoate)	A naturally occuring bioplastic, such as PHA (polyhydroxyalkanoate)	A naturally occuring bioplastic, such as PHA (polyhydroxyalkanoate)
Production process	Chemical synthesis	Bacterial fermentation	Bacterial fermentation	Production in field crop plants
Involvement of GMOs	No	No	Yes Genetically modified microorganism	Yes Genetically modified crop plant
Containment of production process	Contained; closed system	Contained; closed system	Contained; closed system	Open field
Feedstock	Fossil resources	Agricultural biomass, grown for this purpose	Agricultural biomass, grown for this purpose	Sunlight, water, air, other agricultural inputs
Involved industrial sectors	Refineries Chemical industry Plastics processing industry	Farmers Chemical industry Plastics processing industry	Farmers Chemical industry Plastics processing industry	Plant breeders, seed companies Farmers Chemical industry Plastics processing industry

Step 1:
Familiarise yourself with the four options (see description and table on pages 6-7 of the questionnaire)

Step 2:
Scoring: Decide how each appraisal criterion applies to each option.

Step 3:
Repeat step 2 for each criterion

Step 4:
Give a weighting for each appraisal criterion.
Example: Fill in "3" for all criteria that are most important for you.

Step 2:
Give comments to allow insight into your reasoning

	Appraisal criteria	**Options**				**Weighting of appraisal criterion**	
		Conventional chemistry from fossils	Biotechnological production from biomass with				
			Bacteria	GM bacteria	GM plants		
		A	**B**	**C**	**D**		
		***0**: does not apply* ***1**: not realised, false* ***2**:partially realised, true to a certain extent* ***3**: fully realised, true* ***?**: uncertain, depends*				***0**: undecided* ***1**: not important* ***2**: somewhat important* ***3**: very important*	
1	Contributes to saving fossil resources	*0*	*2*	*2*	*2*	*1*	
7	Has low production costs	*3*	*2*	*?*	*?*	*3*	*Depends very much on the feedstock price and downstream pro-cessing*
22	Does not need more than the usual level of stakeholder involvement and stakeholder consultation in decision-making processes	*3*	*3*	*2*	*1*		

Step 2:
Example of scoring: You are of opinion that stakeholder consultations are required for option D, but not for option A and B

Please note: there are no "correct" or "false" answers in this assessment! The main purpose is to map which appraisal criteria you apply in your reasoning, and how the options score for each criterion, according to your own opinion.

16.	Please imagine that a new production process for a certain sort of plastic is to be established, with the goal to produce this plastic in bulk quantities in 2030. A plastic with the desired properties could be made accessible via four different manufacturing routes (Options A-D, see table). Which criteria do you apply in the assessment, and how does each option score for each criterion?

Please refer to the accompanying guide for how to fill in this part of the questionnaire. Please give your own opinion.

	Appraisal criteria ***For the specified option A to D, the option…***	**Options**				**Weighting of appraisal criterion**	**Comments**
		Conventional chemistry from fossils	Biotechnological production from biomass with				
			Bacteria	GM bacteria	GM plants		
		A	**B**	**C**	**D**		
		***0**: does not apply* ***1**: not realised, false* ***2**: partially realised, true to a certain extent* ***3**: realised, true* ***?**: uncertain, depends*				***0**: undecided* ***1**: not important* ***2**: somewhat important* ***3**: very important*	
1	Contributes to saving fossil resources						
2	Reduces the country's dependency on fossil resources (e.g. oil imports, oil prices)						
3	Helps to make industrial chemical production more sustainable						
4	Helps to make agricultural production more sustainable						
5	Strengthens long-term international competitiveness, export position and innovation in the EU chemical industry						
6	Strengthens the EU economy as a whole						
7	Has low production costs						

	Appraisal criteria ***For the specified option A to D, the option…***	**Options**				**Weighting of appraisal criterion**	**Comments**
		Conventional chemistry from fossils	Biotechnological production from biomass with				
			Bacteria	GM bacteria	GM plants		
		A	**B**	**C**	**D**		
		***0**: does not apply* ***1**: not realised, false* ***2**: partially realised, true to a certain extent* ***3**: realised, true* ***?**: uncertain, depends*				***0**: undecided* ***1**: not important* ***2**: somewhat important* ***3**: very important*	
8	Is economically attractive and viable without incentives such as tax exemptions or subsidies						
9	Does not require major adaptation processes from the affected players along the value chain (e.g. new equipment, know-how and processes, altered supply chains)						
10	Can be realised with available state of the art knowledge and technologies						
11	Helps to achieve climate protection goals, because it contributes to the reduction of greenhouse gas emissions.						

12	Is likely to perform better than competing options regarding key environmental impacts such as total energy use, greenhouse gas emissions, etc. This superiority could be demonstrated through e.g. life cycle assessments.						
	Appraisal criteria ***For the specified option A to D, the option…***	**Options**				**Weighting of appraisal criterion**	**Comments**
		Conventional chemistry from fossils	Biotechnological production from biomass with				
			Bacteria	GM bacteria	GM plants		
		A	**B**	**C**	**D**		
		***0**: does not apply* ***1**: not realised, false* ***2**: partially realised, true to a certain extent* ***3**: realised, true* ***?**: uncertain, depends*				***0**: undecided* ***1**: not important* ***2**: somewhat important* ***3**: very important*	
13	Contributes to the structural development of rural areas, and provides a sizable new source of income and employment for farmers						
14	Has a positive impact on agricultural land use (e.g. preservation of agricultural landscape, use of set-aside land)						
15	Favours local, decentralised, small scale agricultural production, local processing plants and small and medium-sized enterprises						

16	Favours large scale agricultural production, centralised processing plants and large companies						
17	Serves customers' and consumers' preferences for goods and products that are produced by sustainable processes						
18	Is considered to be worth paying for by customers and consumers because they perceive that it has unique characteristics which offer value for money						
	Appraisal criteria ***For the specified option A to D, the option…***	**Options**				**Weighting of appraisal criterion**	**Comments**
		Conventional chemistry from fossils	Biotechnological production from biomass with				
			Bacteria	GM bacteria	GM plants		
		A	**B**	**C**	**D**		
		***0**: does not apply* ***1**: not realised, false* ***2**: partially realised, true to a certain extent* ***3**: realised, true* ***?**: uncertain, depends*				***0**: undecided* ***1**: not important* ***2**: somewhat important* ***3**: very important*	
19	Is not considered to require special product information (e.g. labelling, standards, certificates) which would inform customers and consumers about how the product is produced						

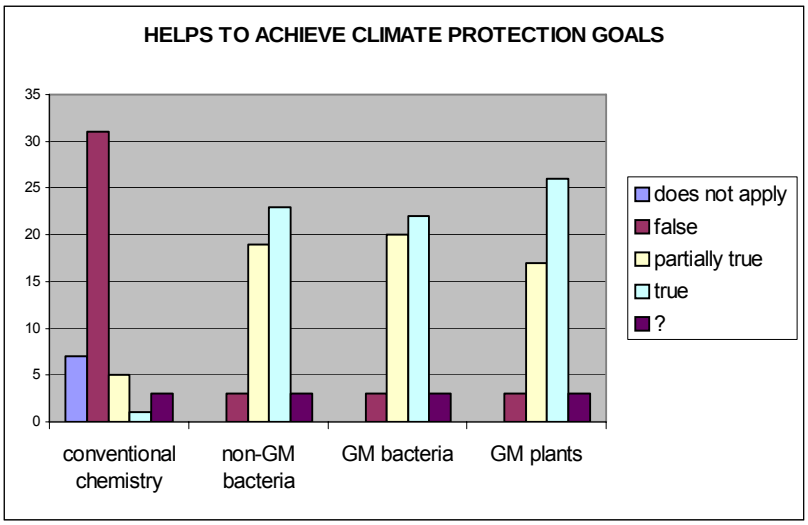
20	Leads to a fair social and regional distribution of benefits and risks (e.g. employment, income, environmental impacts, structural change)						
21	Does not require specific support schemes (e. g. policy priorities, regulations, R&D programmes) in order to be realised						
22	Does not need more than the usual level of stakeholder involvement and stakeholder consultation in decision-making processes						
23	Is deemed favourable because it avoids the use of genetically modified organisms, and thus a variety of undesired and unintended impacts inherent to the use of GMOs						

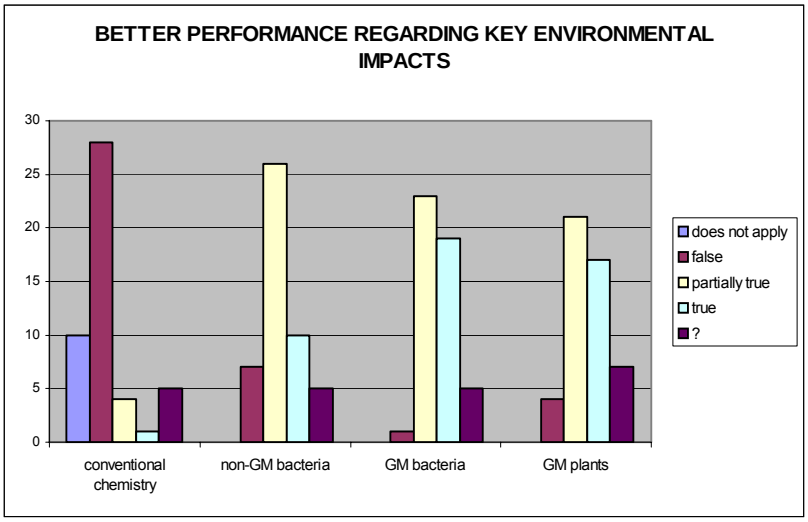
	Appraisal criteria ***For the specified option A to D, the option…***	**Options**				**Weighting of appraisal criterion**	**Comments**
		Conventional chemistry from fossils	Biotechnological production from biomass with				
			Bacteria	GM bacteria	GM plants		
		A	**B**	**C**	**D**		
		***0**: does not apply* ***1**: not realised, false* ***2**: partially realised, true to a certain extent* ***3**: realised, true* ***?**: uncertain, depends*				***0**: undecided* ***1**: not important* ***2**: somewhat important* ***3**: very important*	

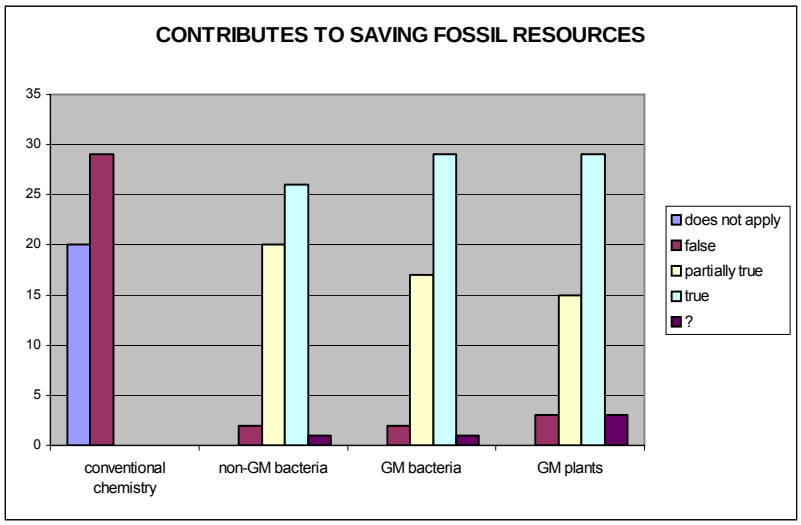
24	Uses genetically modified organisms which could possibly lead to undesired and unintended impacts; however these can be effectively prevented and managed						
25	Other appraisal criteria; please specify						
26							
27							
28							
29							
30	All in all, according to my personal assessment, I rank the options in the order:						
		1 = most favourable option; 4 = least favourable option					

Thank you very much for your participation!

Appendix 15: Additional results from the BREW survey






CONTRIBUTES TO SAVING FOSSIL RESOURCES
35
30
25
20
15
10
5
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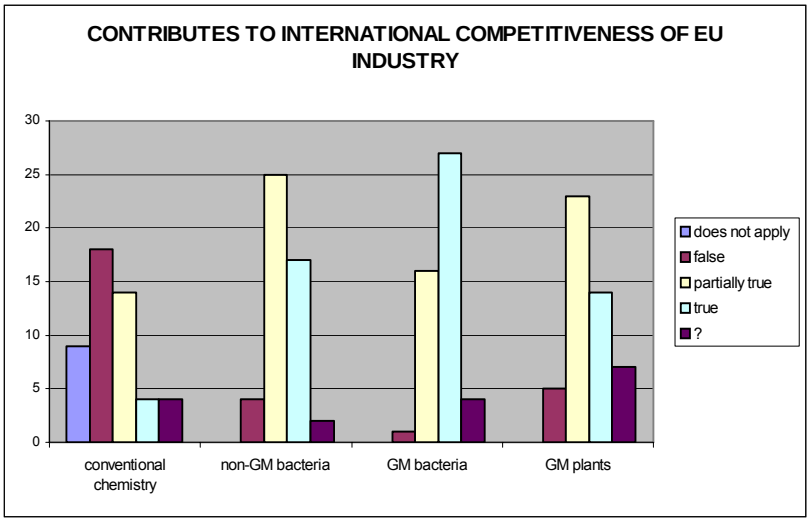
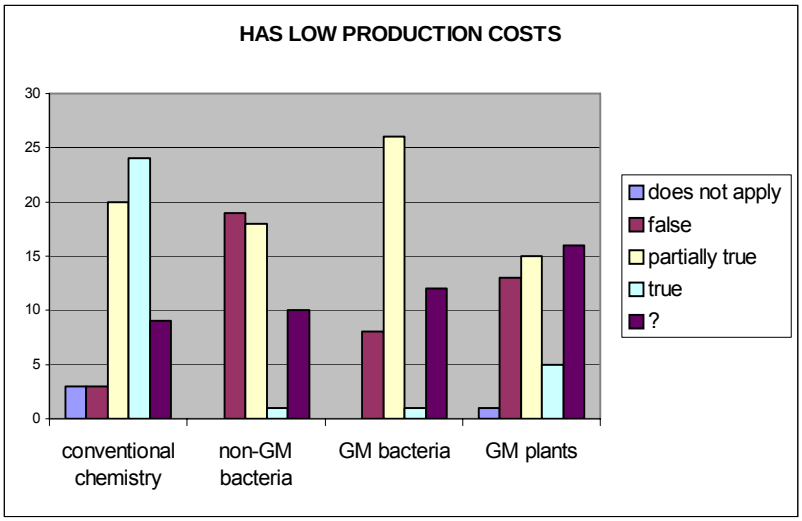
non-GM bacteria
GM bacteria
GM plants
does not apply
false
partially true
true
?


CONTRIBUTES TO INTERNATIONAL COMPETITIVENESS OF EU INDUSTRY
30
25
20
15
10
5
0
conventional chemistry
non-GM bacteria
GM bacteria
GM plants
does not apply
false
partially true
true
?


HAS LOW PRODUCTION COSTS
30
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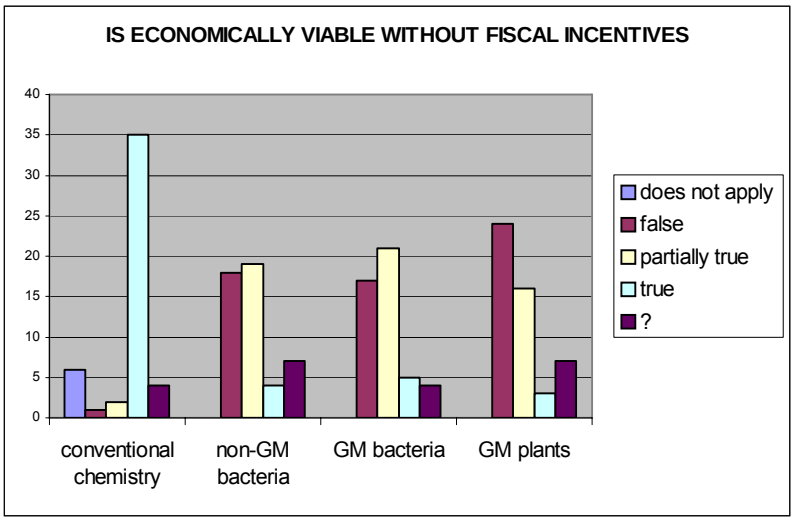
conventional chemistry
non-GM bacteria
GM bacteria
GM plants
does not apply
false
partially true
true
?


IS ECONOMICALLY VIABLE WITHOUT FISCAL INCENTIVES
40
35
30
25
20
15
10
5
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GM bacteria
GM plants
does not apply
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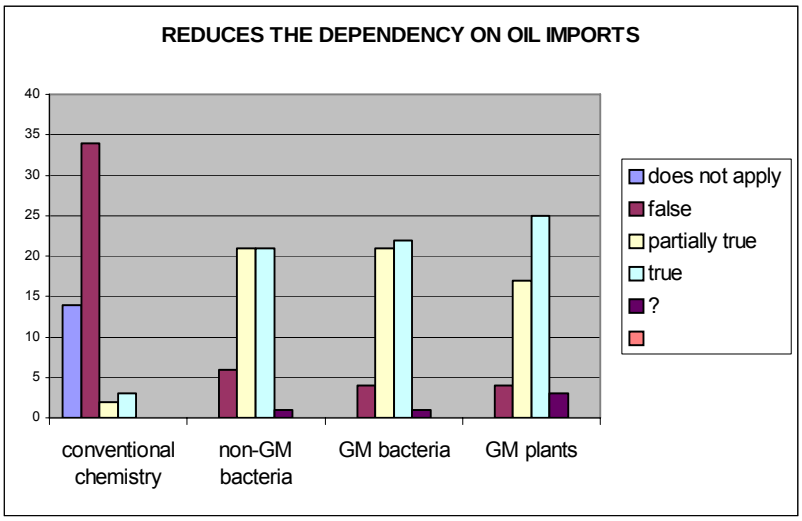
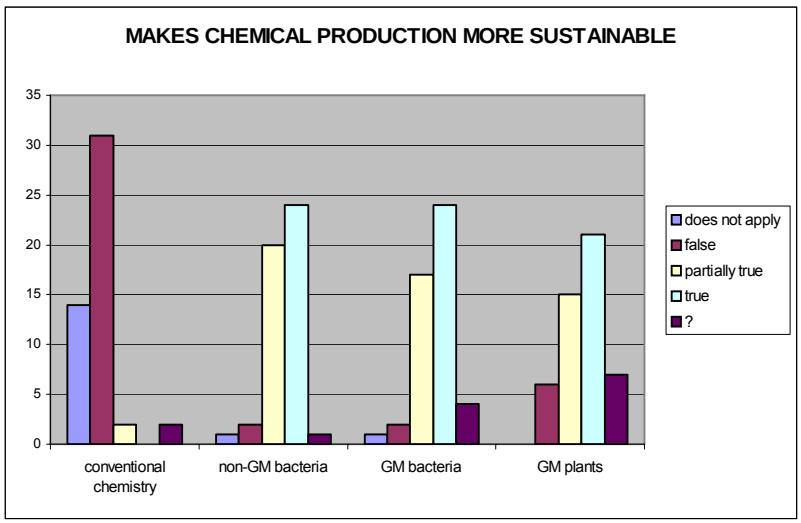
partially true
true
?


REDUCES THE DEPENDENCY ON OIL IMPORTS
40
35
30
25
20
15
10
5
0
conventional chemistry
non-GM bacteria
GM bacteria
GM plants
does not apply
false
partially true
true
?


MAKES CHEMICAL PRODUCTION MORE SUSTAINABLE
35
30
25
20
15
10
5
0
conventional chemistry
non-GM bacteria
GM bacteria
GM plants
does not apply
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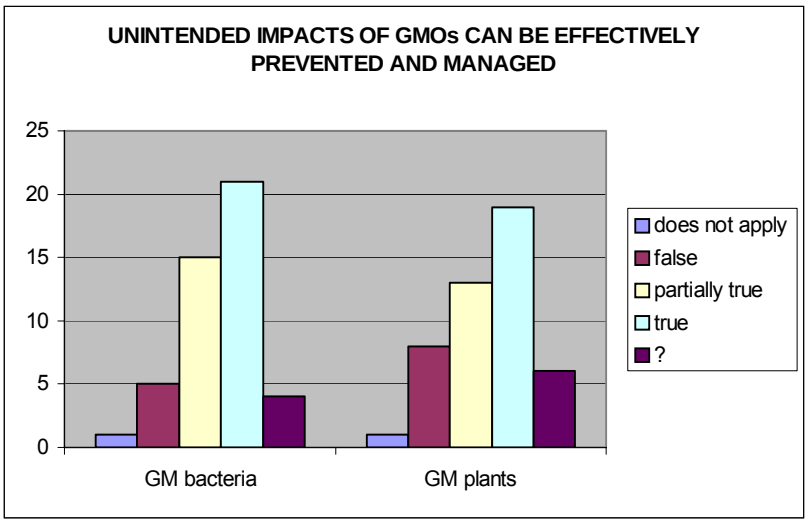
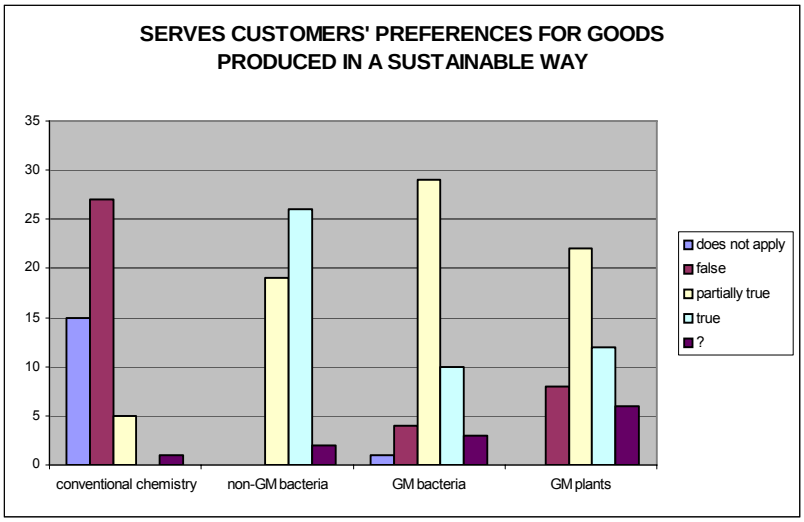
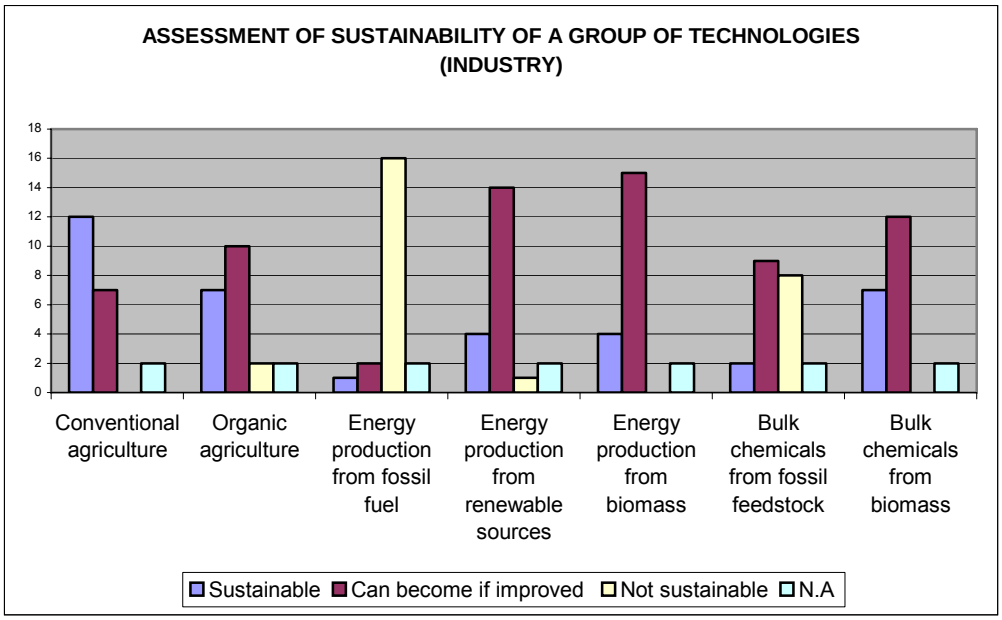
partially true
true
?

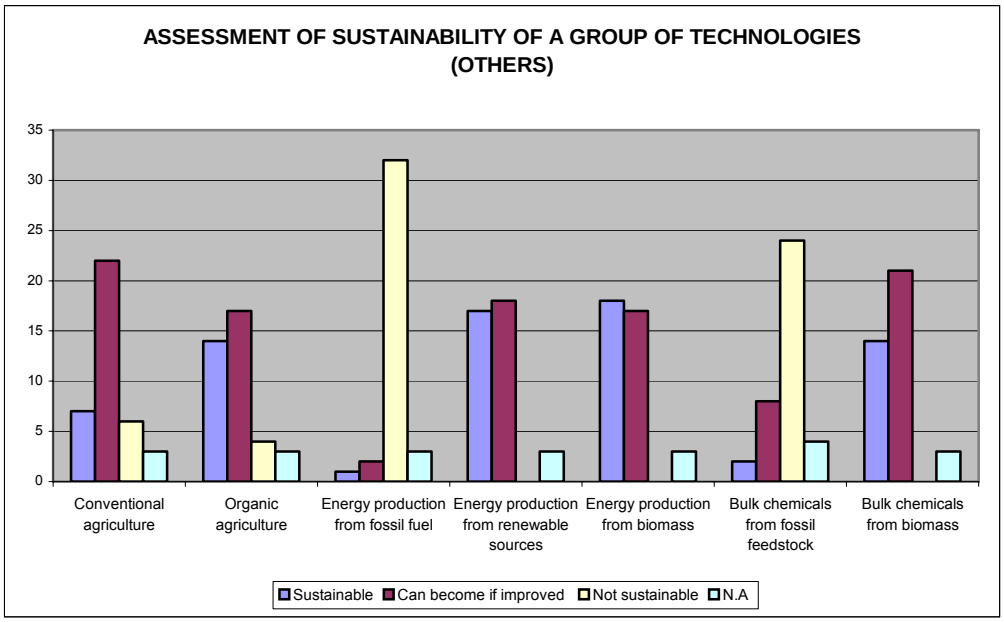

UNINTENDED IMPACTS OF GMOs CAN BE EFFECTIVELY PREVENTED AND MANAGED
25
20
15
10
5
0
GM bacteria
GM plants
does not apply
false
partially true
true
?


SERVES CUSTOMERS' PREFERENCES FOR GOODS PRODUCED IN A SUSTAINABLE WAY
35
30
25
20
15
10
5
0
conventional chemistry
non-GM bacteria
GM bacteria
GM plants
does not apply
false
partially true
true
?

Disaggregated analysis

In order to separate the 'insider' views from the views of the rest of the sample, considered as a more realistic 'proxy' of the general public, the sample has been split in two components: 'industry' (N = 21), including representatives of industrial companies, and 'other respondents' (N = 38). The results of the survey have been then analysed separately; indeed considerable differences emerged between the two components. Such differences already emerge concerning the respondents' views about the general context and the sustainability of other technologies.

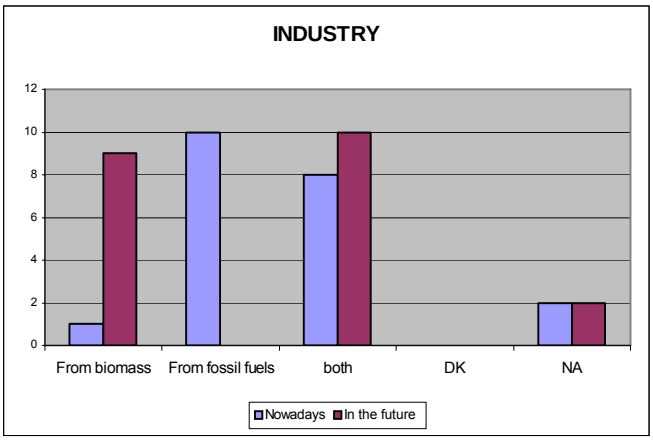


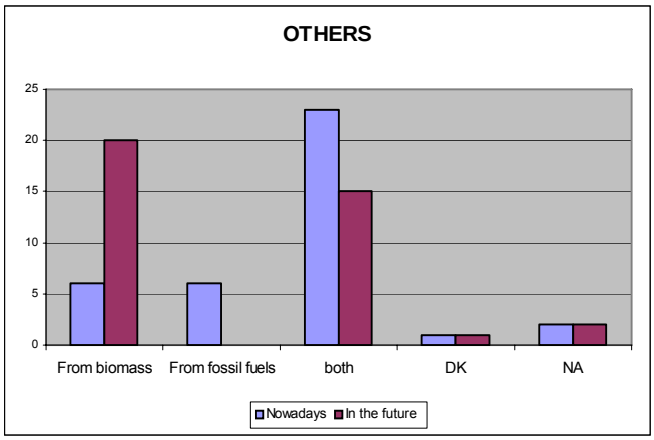


One of the most apparent differences concerns the assessment of conventional agriculture, which is seen as much more 'sustainable' by the respondents in the 'industry' group. Conversely, renewable energies are seen as more 'sustainable' by the non-industry group. Concerning energy production from biomass, the industry group appears more cautious assuming that significant 'improvements' are required to ensure sustainability. Another major difference is about conventional chemical production from fossil feedstock, which is seen as not sustainable by 63% of the 'non-industry' respondents, compared to 38% of the 'industry' group. Finally, the two groups express rather similar views as concerns bulk chemicals production from biomass, though the 'non-industry' group is slightly more optimistic about the sustainability of this technology. No significant differences emerge concerning the importance attached to fundamental changes in some technological areas, except for the shift from conventional to organic agriculture.

Considerable discrepancies start to appear when it comes to the core issue of the survey, technological options in chemicals production. A much more conservative attitude is expressed by the 'industry' group toward the idea of shifting from fossil to biomass feedstock (48% would maintain fossil fuel in the present compared to 16% for the 'others' group), though the difference seems to even out when it comes to 'the future'.

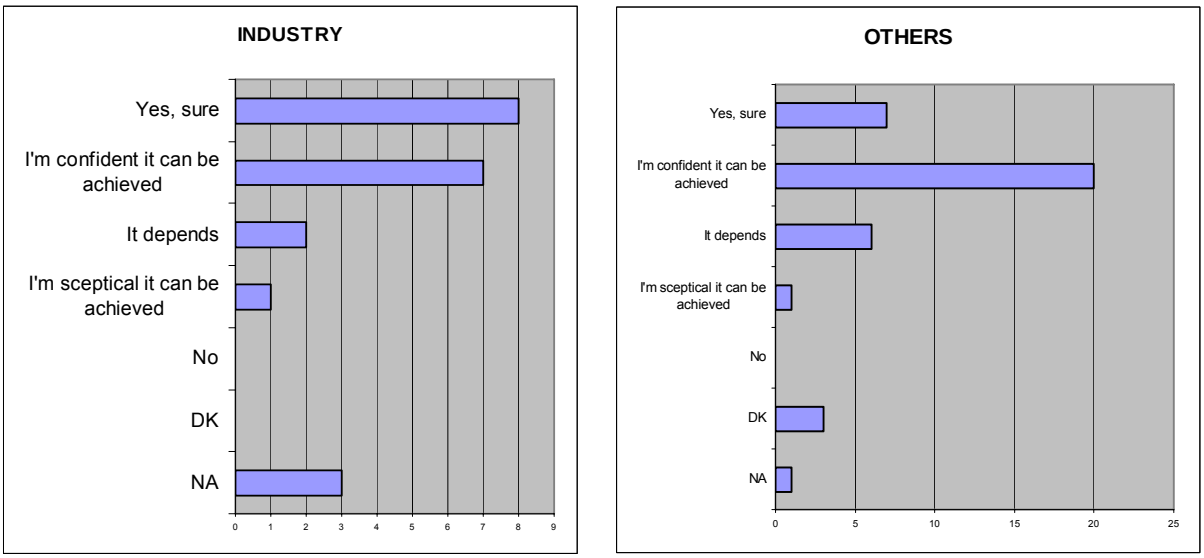
Bulk chemicals from biomass or fossil feedstock?





No significant differences are found for the following questions 11 (reduction of greenhouse gas emissions) and 12 (key environmental impacts), while concerning the respondents' attitudes to risk inherent in biotechnological production (question 23 and 24), differences are apparent. The 'industry' group shows a much more optimistic attitude (38% is 'sure' that the risks will be controlled compared to 18% for the other group). However, optimism appears overwhelming in both groups.

Will the risks inherent in the use of biotechnology for manufacturing chemicals from biomass be successfully managed?



Again, the two groups show similar (definitely optimistic) patterns concerning the development perspectives of the new technology in terms of innovation and economic growth (question 14), while as concerns its potentialities to revitalise the petrochemical industry (question 15) the attitudes are more mixed and the rate of 'don't know' in the 'others' group reaches 50%. However, this outcome is inherent in the 'outsider' position of this group.

Where the positions of the two groups appear very distant is at question 16, when it comes to weighing the criteria used to appraise the four technological options for chemicals production. Here the different value sets clearly emerge as shown by the following comparison of the (implicit) rankings of the criteria made by the two groups:

INDUSTRY	OTHERS
1. Has low production costs (16.7). 2. Is economically attractive and viable without incentives such as tax exemptions or subsidies (16.8). 3. Strengthens long-term international competitiveness, export position and innovation in the EU chemical industry (16.5). 4. Is likely to perform better than competing options regarding key environmental impacts such as total energy use, greenhouse gas emissions, etc. This superiority could be demonstrated through e.g. life cycle assessments(16.12). 5. Does not require specific support schemes (e.g. policy priorities, regulations, R&D programmes) in order to be realised (16.21) 6. Contributes to saving fossil resources (16.1). 7. Serves customers' and consumers' preferences for goods and products that are produced by sustainable processes (16.17). 8. Strengthens the EU economy as a whole (16.5) 9. Helps to achieve climate protection goals, because it contributes to the reduction of greenhouse gas emissions (16.11). 10. It is not considered to require special product information (e.g. labelling, standards, certificates) which would inform customers and consumers about how the product is produced (16.19)	1. Helps to achieve climate protection goals, because it contributes to the reduction of greenhouse gas emissions (16.11). 2. Contributes to saving fossil resources (16.1). 3. Is likely to perform better than competing options regarding key environmental impacts such as total energy use, greenhouse gas emissions, etc. This superiority could be demonstrated through e.g. life cycle assessments(16.12). 4. Reduces the country's dependency on fossil resources (e.g. oil imports, oil prices) (16.2.). 5. Helps to make industrial chemical production more sustainable (16.3.). 6. Has a positive impact on agricultural land use (e.g. preservation of agricultural landscape, use of set-aside land) (16.14) 7. Contributes to the structural development of rural areas, and provides a sizable new source of income and employment for farmers (16.13) 8. Strengthens long-term international competitiveness, export position and innovation in the EU chemical industry (16.5) 9. Uses genetically modified organisms which could possibly lead to undesired and unintended impacts; however these can be effectively prevented and managed (16.24.). 10. Helps to make agricultural production more sustainable (16.4).

The ‘industry’ group expectably attaches much more importance to economic and legal criteria (ranking 1, 2, 3, 5, 8, 10) while in the ‘generic’ component of the sample the environmental criteria play a dominant role (1, 2, 3, 5, 9, 10) and considerable attention is given to aspects related to agriculture and farmers’ conditions (6, 7) that are totally ignored by the former group. Finally, the geopolitical factor (dependency on oil imports) seems not to be relevant for the industry group, while it ranks 4 for the rest of the sample.

The ranking of the four technological options for bulk chemicals production is slightly different for the two groups, but when measured by one overall index it results in the same order of preferences which obviously coincides with the order found for the sample as a whole (GM bacteria, bacteria, GM plants, conventional chemistry). However, it is interesting to notice that no one in the ‘generic’ sample ranks first the option ‘GM plants’.