Today's and Tomorrow's Bio-Based Bulk Chemicals From White Biotechnology

A Techno-Economic Analysis

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Received March 28, 2006; Revised July 17, 2006; Accepted July 20, 2006

Abstract

Little information is yet available on the economic viability of the production of bio-based bulk chemicals and intermediates from white biotechnology (WB). This paper details a methodology to systematically evaluate the techno-economic prospects of present and future production routes of bio-based bulk chemicals produced with WB. Current and future technology routes are evaluated for 15 products assuming prices of fermentable sugar between $70 \notin t$ and $400 \notin t$ and crude oil prices of US \$25/barrel and US \$50/barrel. The results are compared to current technology routes of petrochemical equivalents. For current state-of-the-art WB processes and a crude oil price of US \$25/barrel, WB-based ethanol, 1,3-propanediol, polytrimethylene terephthalate and succinic acid are economically viable. Only three WB products are economically not viable for future technology: acetic acid, ethylene and PLA. Future-technology ethylene and PLA become economically viable for a higher crude oil price (US \$50/barrel). Production costs plus profits of WB products decrease by 20–50% when changing from current to future technology for a crude oil price of US \$25 per barrel and across all sugar prices. Technological progress in WB can thus contribute significantly to improved economic viability of WB products. A large-scale introduction of WB-based production of economically viable bulk chemicals would therefore be desirable if the environmental impacts are smaller than those of current petrochemical production routes.

Index Entries: White biotechnology; industrial biotechnology; bulk chemicals; economic analysis; future technology; fermentation; generic approach; 1,3-propanediol.

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Introduction

During the last few years, considerable progress has been made in biotechnology research, and further major scientific and technological breakthroughs are expected for the future. The first large-scale industrial applications of modern biotechnology have been the areas of food and animal feed production (agricultural/green biotechnology) and of pharmaceuticals (medical/red biotechnology) (1). In contrast, the production of organic compounds by means of fermentation or enzymatic conversion (so-called white biotechnology [WB]*) on a large-scale is still in its infancy. Enzymatic conversion is excluded from this paper because the number of bulk chemicals that can be produced by fermentation is much larger (2). In principle, WB can be applied to convert bio-based or petrochemical feedstocks such as methanol. Bio-based feedstocks are the default for WB and petrochemical feedstocks for WB are not covered in this paper.

Most industrial activity has so far been centred on the production of bio-ethanol for fuel use, for example by Archer Daniel Midlands in the United States and Iogen in Canada (*3*) as well as by COPERSUCAR in Brazil (*4*). NatureWorks is the first company producing a bio-based polyester, polylactic acid (PLA), in a large industrial plant (*5*) in Nebraska, and DuPont is currently building a plant for the production of 1,3-propanediol (PDO) from maize-based glucose in Tennessee, expected to be operational in 2006. In Europe, practically all large chemical companies are exploring the possibilities for the production of chemicals by means of WB and they are partly developing industrial processes for selected, mostly higher-value products (*1*). Moreover, the EU bio-fuels directive (*6*) is expected to boost the production volumes of bio-ethanol in the WB sector.

Very little data are publicly available on the techno-economic potentials of WB-based chemicals because of the sensitivity of this information among competitors and because WB is still an emerging technology. Some publications have analyzed the potentials and barriers to the production of WB-based chemicals in general (7-9) and many publications and reports deal with technical aspects of specific process steps such as fermentation and downstream processing. Some detailed techno-economic analyses have been produced by SRI Consulting (e.g., ref. 10) but these are multiclient studies and are therefore not publicly available. Of the few publications on the techno-economics of WB-based products almost all have focused on a single product: most predominantly on ethanol for fuel use (e.g., refs. 11-13), but also on ABE (14) and succinic acid (15,16). Methodologies and background assumptions differ between these studies and the results are not easily compared. Additionally, most available analyses study current technologies and do not account for possible future technological progress. Against this background, it is the aim of this article to assess the economic viability of current and future technologies for producing bio-based bulk chemicals using white biotechnology.

^{*}In the United States, white biotechnology is referred to as industrial biotechnology.

A general problem of process analyses—especially when concerning emerging technologies—is the confidentiality of process data. To overcome this problem, this paper presents and applies a generic approach that circumvents confidentiality issues by allowing to estimate the economic viability of WB production processes based on generic key data, a principle already proposed by (16,17). The methodology allows a systematic evaluation of present and future processing routes of WB-based bulk chemicals. Additionally, economic analyses were performed using confidential data provided by companies and institutes and by combining the basic information from the production cost estimates by SRI (e.g., ref. 10) with uniform assumptions as applied in this study.

After having discussed the generic approach, a detailed case study is presented on 1,3-propanediol. We proceed to calculate and discuss the current and future economics of 15 WB chemicals and compare them to datasets from industry and petrochemical equivalents. These product-byproduct analyses were carried out for variable sugar prices and a crude oil price of US \$25/barrel, with a sensitivity analysis for US \$50/barrel.

This paper focuses on the economics of WB-based bulk chemicals, drawing on detailed data as presented in the EU project "BREW" (2). Based on this project and as an extension to this paper, Dornburg et al. perform an evaluation of the technical, economic and market potentials of these WB products including scenarios with changing crude oil prices until 2050 (18). As a complement to this paper, we moreover apply the generic approach to prepare a systematic comparison of *environmental* impacts across products and for different sources of fermentable sugar (19).

Methodology

Methodological Background

A generic approach is a method allowing standardized comparisons between different processes based on a small number of components. Many calculations can then be carried out based on a small number of input data. Because of the very limited availability of process data for WB processes, a specific generic approach has been developed. This generic approach allows an *ex ante* estimation of the economic viability of biotechnological processes for which pilot plant or lab scale data do not yet exist or for which process data are not publicly available. We applied this method to processes representing the current state-of-the-art as well as future technology. The results from this generic approach were compared to results for WB products calculated using industry data and they were also compared to petrochemical equivalents.

The start of the generic approach was the preparation of a process flow diagram of the bioprocess, which converts fermentable sugar to the target WB chemical. These process flow diagrams contained standard modules (e.g., fermentation, ultrafiltration, evaporation). For each process flow diagram representing one production route, the mass balance containing the quantities of all inputs and outputs at the level of unit processes was determined (*see* "Process Design of WB Routes" and "Technology Assumptions for WB Routes"). On this basis, the costs related to all inputs and the investment costs were estimated and the overall production costs calculated (*see* "Process Economics Methodology"). As an alternative, the information from the mass balance can be used to perform an *environmental* assessment, which is the topic of a separate publication (*see* ref. 19).

In order to ensure the comparability of the results, a common database for process inputs was used for all calculations. This database consists of market prices for chemicals, auxiliaries and utilities as well as prices for fermentable sugar (see "Prices of Fermentable Sugars" and "Prices of Utilities and Auxiliaries").

Functional Unit and Product Selection

The purpose of this paper is to estimate overall production costs for organic bulk chemicals at the factory gate. Therefore, the functional unit was 1⁺ ton of organic chemical at the factory gate. Factories were assumed to be dedicated large-scale installations because of the advantage of economies of scale of large processes, which outweigh the biomass collection costs (20). We make the simplifying assumption that there is only one main product: the WB chemical. This simplification allows a consistent comparison between different chemicals and an overview of the current and future techno-economic potential for WB chemicals.

The selection of products in this paper was based on three criteria: (1) the fermentation process was considered feasible either in literature or by a panel of experts,* (2) basic data on the stoichiometry of the fermentation process was available, and (3) the chemicals or intermediates studied had the potential to be used in bulk quantities, i.e., a production of at least 200 kilotons (kt) per year in Western Europe was envisaged for the medium or long term. As shown in Table 1, current production capacities of the petrochemical equivalents of the selected WB chemicals exceed this value by far. The application of these criteria has resulted in the following selection of products: PDO, acetic acid, acrylic acid, adipic acid, butanol (from the ABE process), ethanol, citric acid, lysine, lactic acid, polyhydroxyalkanoates (PHA), and succinic acid. Additionally, several products were considered that are formed by chemical conversion of a product included in the previous list: polycondensation of lactic acid results in PLA, that of PDO and purified terephthalic acid in polytrimethylene terephthalate (PTT); ethanol is dehydrated to yield ethylene; ethanol and lactic acid are converted to

^{*}The panel consisted of representatives from A&F, BP Chemicals, Degussa, DSM Research, DuPont, NatureWorks, Novozymes, Roquette Frères, Shell International Chemicals and Uniqema. These are the industry partners of the BREW project (2).

⁺All tons referred to in this article are metric tons (ca. 1.102 short tons).

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Product	Installed capacity (kt/yr)	Year	Reference	Equivalent for WB-based
Acetic acid	1400	2000	22	Acetic acid
Acrylic acid	820	1999	22	Acrylic acid
Adipic acid	1000	1999	22	Adipic acid
Butanol	930	1999	22	Butanol
Caprolactam	1100	1999	22	Caprolactam
Ethanol ^a	580	1998	22	Ethanol
Ethyl acetate	310	1999	22	Ethyl lactate
Ethylene	22,200	2000	22	Ethylene
Maleic anhydride	380	1999	22	Succinic acid
PDO/PTT	No data	No data	No data	PDO/PTT
Polyethylene	12,900	2000	Based on 22	Polyhydroxyalkanoates
Polyethylene terephthalate	2,170	2004	23	Polylactic acid

Table 1
Production Capacities of the Petrochemical Equivalents
of the 15 White Biotechnology (WB) Products in Western Europe

^{*a*}The installed capacity of bio-based production of ethanol is 560 kt/yr (22). This is not included in the table because bio-based ethanol is mostly used as fuel, whereas the ethanol used in the chemical industry predominantly stems from petrochemical production processes. PDO, 1,3-propanediol; PTT, polyethylene terephthalate.

ethyl lactate; and lysine is transformed into caprolactam via chemical cyclization. Table 1 shows the production volumes of the petrochemical equivalents of the WB products. Lysine and lactic acid were excluded because they have no petrochemical equivalents; both are used as intermediates, e.g. for caprolactam and PLA, but may also have stand-alone applications such as poly- ϵ -lysine (*see* ref. 21).

Total petrochemical production volume in Western Europe amounted to 46 million tons in 1999 (derived from refs. 22,24), showing that a significant portion of the market was included in this study.

Process Design of WB Routes

Separate process flow diagrams were made for current and future technologies, both with respect to the fermentation processes and downstream processing for product separation and purification. All process flow diagrams (prepared at the level of unit processes) consisted of the following sections (*see* Fig. 1): seed and inoculum trains (provision of microorganism), fermentation (conversion of sugar to the target product and by-products), filtration (removal of solid by-products), and downstream processing (several steps, to purify the target product). The material inputs to the system were fermentable sugar, water, nutrients, auxiliary substances and utilities such as electricity and steam. The outputs were the target product as well as solid waste and wastewater.



Fig. 1. Simplified flowsheet as used in the generic approach.

Technology Assumptions for WB Routes

When preparing the mass balance, the mass flows of all compounds were estimated based on the following key parameters: yields, productivity and broth concentration of the fermentation step (*see* Table 2). The broth concentration* determines the amount of water in the broth and therefore influences the energy required in downstream processing. Together with productivity,[†] it determines the residence time as well as the size of the fermentation equipment. The yield[¶] influences not only the required input of fermentable sugar but also the amount of waste biomass produced. Waste biomass is separated from the product stream by means of an ultrafiltration step that immediately follows fermentation. The waste biomass is dried and is then burnt for steam production. Process water is recycled wherever possible in order to avoid excessive consumption.

As part of the generic approach, assumptions were made for the key parameters of current and future technology regarding fermentation and downstream processing (Table 2). Although both continuous and batch processes were assumed for current technology, only continuous processes were assumed for the future. Current technology calculations rely on data from industrial units, pilot plants, or laboratory experiments; future technology calculations rely on two to three decades of successful research and

^{*}Broth concentration is defined as the mass of product relative to the volume of water in the fermentation broth (in g/L).

⁺Productivity is defined as the mass of the product divided by the volume of fermentation broth per unit of time needed to produce this amount in $(g/[L\cdoth])$.

 $^{{}^{}l}\!Yield$ is defined as the mass of the product divided by the mass of the fermentable sugar (in g/g)

oductivity, and Yields hnology		uctivity Yield /(L·h) g product/g glucose Reference	0.36 0.42 14,25,26	15 0.50	0.15 0.50 $27,28$	15 0.90	10 0.72	0.42 0.17 29	10 0.47	2.2 0.46 17,30,31	50 0.47	20 0.95	1.7 0.34 32	10 0.63	1.67 - 6 0.41 33	15 0.54	3.0 0.35 34	10 0.43	1.8 0.88 10,35	15 1.01	
Table 2 and Key Data on Concentration, Pro entation for Current and Future Tecl	on Broth	3atch/ concentration Prod continuous g/L g/	sont. 20	cont. 45	$\frac{18}{2}$	cont. 50	cont. 50	20 20	cont. 40	cont. 100	cont. 130	cont. 180	atch 100	cont. 140	oatch, cont. 100	cont. 100	atch 150	cont. 150	batch 80	cont. 150	dial. DH A mattheodory
Type of Fermentation . of Ferme	Type of fermentati	Today/ Aerobic/ E cuture anaerobic c	Today anaer. c	Future anaer. c	Today anaer. b	Future anaer. c	Future anaer. c	Today aerobic b	Future aerobic c	Today anaer. c	Future anaer. c	Future anaer. c	Today aerobic b	Future aerobic c	Today aerobic b	Future aerobic c	Today aerobic b	Future aerobic c	Today anaer. b	Future anaer. c	lothand. PDO 1 2-manual
		7 Product f	1 ABE (butanol)		2 Acetic acid		3 Acrylic acid	4 Adipic acid	1	5 Ethanol	- •	6 Lactic acid	7 Lysine		8 PDO		9 PHA		10 Succinic acid		A BE sector button

development (R&D; *see* Table 2). The resulting future process data represent a possible upper level of technological feasibility.

For current fermentation technology, the values of yields, broth concentration and productivity in Table 2 were based on published data. Any fermentable sugar not converted to the target product was split between by-products, waste biomass and CO_2 emissions according to published data (10,14,17,25–35). Regarding lactic acid and acrylic acid, generic calculations were only carried out for future technology because industrial data for producing lactic acid according to today's technology were available (5) and because the production of acrylic acid is still in a very early stage of R&D.

For future fermentation processes, we assumed a yield of 90 mol-% of the maximum theoretical yield. The remaining fermentable sugar (10 mol-%) is converted into waste biomass and CO₂ only, with an assumed carbon ratio of 1:2 for aerobic and 1:1 for anaerobic processes.* This implies that fermentation of by-products can be suppressed, which will most likely require genetic modification of the micro-organism. Future productivities were based on citric acid and ethanol as two representatives of advanced aerobic and anaerobic fermentation processes that have improved faster than other substances because of higher R&D efforts. Their future upper productivity levels were estimated by experts to reach 10 g/L/h for citric acid⁺ and 50 g/(L·h) for ethanol.[¶] Productivity of the other chemicals was assumed to approach the horizon values of citric acid for aerobic and ethanol for anaerobic fermentation, representing a comparable level of ambition. Future broth concentrations of continuous processes were estimated to be in the range of today's end-of-batch values due to interactions between productivity and concentration:

- Future technology will rely on continuous fermentation at the point of maximum productivity of the micro-organism with *in situ* removal of the product. The maximum productivity for current processes occurs at approximately half the maximum batch concentration.
- For future technology, the broth concentration corresponding to this maximum productivity was assumed to be increased by a factor of two, thereby resulting in broth concentrations in the range of current batch fermentation.

^{*}This estimate is based on detailed calculations on the carbon splitting of four anaerobic and four aerobic fermentation processes. The aerobic processes have ratios around 1:2. For anaerobic processes the spread is much larger, because less metabolic CO_2 should be formed than for aerobic processes we assume a ratio of 1:1.

[†]Productivities as high as 5 g/(L·h) have been reported (*36*), so an increase by a factor of two resulting in 10 g/(L·h) appears feasible within 20–30 yr.

[§]Some authors (37,38) reported productivities even higher than 50 g/(L·h), but with current productivities around 2 g/(L·h), an increase beyond 50 g/(L·h) on an industrial scale appeared unlikely within 20–30 yr.

	Today's technology	Future technology
Adsorption	—	Lysine
Crystallization	Succinic (10), Adipic (39)	Succinic, adipic
Distillation	PDO (33), Ethanol (30), ABE (14)	Ethanol, ABÊ
Electrodialysis	Succinic (15), Acetic (40)	Succinic, lactic, acetic, adipic
Enzymes	PHA (41)	РНА
Extraction	Acetic (42), PHA (41)	Acetic ^{<i>a</i>} , acrylic
Gas stripping	ABE (26)	ABE
Ion-exchange	Lysine (32)	_
Pervaporation	Ethanol (43)	PDO, ethanol, ABE

Table 3 Types of Downstream Processing Used for Separation in Today's and Future Technology for the White Biotechnology Products

^{*a*}For acetic acid future technology, there are not only flowsheets on extraction and electrodialysis, but also one that combines both of these separation technologies.

 $PDO, 1, 3\-propanediol; ABE, acetone-butanol-ethanol; PHA, polyhydroxyalkanoates.$

The values assumed for these key technical parameters were critically reviewed by project partners and represent the technical potential after 20–30 yr of R&D. However, predicting future key technical parameters always involves uncertainty. We have therefore carried out an exemplary sensitivity analysis for ethanol with a significantly lower productivity to assess its influence on economic viability (*see* "Sensitivity to Key Technical Parameters").

Table 3 presents an overview of the types of downstream processes that were used to separate the products of current and future technology. Polylactic acid, polytrimethylene terephthalate, ethylene, ethyl lactate, and caprolactam do not appear in Table 3 because they are derived by chemical conversion from one of the WB products listed in this table.

The type of downstream processing for today's technology was derived from literature (*see* Table 3). Assumptions for future technology separation processes were based on a number of considerations:

- Precipitation was not considered viable for large-scale production because it involves the use of large amounts of chemicals and leads to low-value by-products such as gypsum and/or wastewater with high salt loads.
- Extraction and adsorption were considered acceptable future options because of the potential use of "green solvents" with clearly lower environmental impacts (e.g., in terms of carcinogenic and toxic effects) compared to current solvents.
- Membrane processes such as pervaporation, electrodialysis and ultrafiltration were taken into account due to their (expected) low energy use. However, a significant amount of R&D will often still be

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Unit process	Amount	Unit
Fermentation		
Sterilization	0.1	kg steam/kg fermentation medium
Agitation	0.5	kW power/m ³ fermentation volume
Agitation and aeration	3.0	kW power /m ³ fermentation volume
Downstream processing		
Membrane filtration		
 Microfiltration 	2.0	kWh power /m ³ permeate
 Ultrafiltration 	5.0	kWh power /m ³ permeate
 Diafiltration 	5.0	kWh power /m ³ permeate
 Nanofiltration 	7.0	kWh power /m ³ permeate
 Reverse osmosis 	9.0	kWh power /m ³ permeate
Electrodialysis	0.1	kWh power /equivalent ^a
Evaporation of water,		
single stage	1.2	kg steam/kg evaporated
8 8	0.04	kWh power/kg evaporated
Evaporation of water,		1 0 1
multi-stage	0.5	kg steam/kg evaporated
. 8 .	0.005	kWh power /kg evaporated
Distillation	1.3 * product's heat of evap.	kg steam/kg evaporated

Table 4 Key Data on Specific Energy Use of Unit Processes

^{*a*}An equivalent is here considered as the number of dissociations that the acid can undergo, i.e., the number of protons it can give up.

necessary to put these membrane processes into use on an industrial scale.

• Today's as well as future technology assumed single step evaporation up to a water-product ratio of 5:1 for evaporation processes; for larger proportions of water, double-effect evaporation was assumed and increased investment costs were accounted for.

Energy Use

The process energy for the system covered in the generic approach was determined by multiplying the mass and volume throughputs by the estimated specific energy use for each process step. The specific process energy as shown in Table 4 was estimated based on literature, then calibrated (for a detailed description of the procedure, *see* ref. 2).

Process Economics Methodology

The economic analysis for WB chemicals was performed for an assumed plant capacity of 100 kt/yr, which was a compromise in view of economies of scale on the one hand and transport costs for the bio-feedstocks on the other. This scale was considered representative for a WB plant, but larger scales are also possible and a sensitivity analysis was carried out to assess the influence of plant size on economic viability (*see* "Sensitivity to Economic Parameters"). Petrochemical processes were calculated for current plant sizes, which can be clearly larger than 100 kt depending on the product (*see* "Petrochemical Process Data").

All cost calculations were based on investments for building a new plant in Western Europe, with calculations carried out in \in_{2000} . The investment (Total Fixed Capital [TFC]) and labor requirements were estimated by DSM by applying their so-called *Functional Unit Method* (44). These calculations were carried out for each generic WB route based on the individual product flow sheet, mass and energy balance (*see* ref. 2 for individual numbers). We used market prices for petrochemical feedstocks and auxiliaries, the prices of fermentable sugar were set exogenously (*see* "Prices of Fermentable Sugars").

The procedure for the economic assessment (*see* Fig. 2) is in line with standard business economics: first, variable costs (feedstock, auxiliaries/catalysts, by-products, utilities, waste treatment) and fixed costs (supplies, labor) were added to obtain the total direct operating costs. Second, taxes, insurance fees and plant overhead were added to this figure as well as an allowance for marketing, administration, and R&D. And finally, the so-called capital charge, representing the total of depreciation and profits, was added. The final result is the production cost plus profits (PCPP; also known as profited production cost) which is a proxy for the market price. The capital charge was calculated by multiplying the total fixed capital charge of 30% was used, partially accounting for contingency (*see* "Sensitivity to Economic Parameters" for a sensitivity analysis). Value-added tax was not included in the calculations.

A given WB product was considered economically viable if its PCPP was lower than the market price or the PCPP of its petrochemical counterpart. The real market price of the WB product may be higher or lower than its PCPP depending on demand and supply:

- The PCPP of a WB product is usually substantially lower than its market price if the WB product is new on the market and if it is used for niche applications. Possible reasons are that the profit made is higher, the *real* capacity of the production facilities is clearly lower than 100 kt/yr, the process is not optimized and/or continuous operation cannot be ensured.
- The PCPP of the WB product can also be higher than the market price. This is particularly the case if the WB product is chemically identical with a petrochemical product that has been manufactured for decades via an established production route. Such petrochemical processes can be economically superior because of the advantageous economies of scale and/or production in depreciated plants.



Fig. 2. Procedure to calculate production costs plus profits (PCPP).

WB Industrial Process Data

For some bio-based processes, confidential information was made available to us by companies and research institutes for the biotechnological plant as a whole. These confidential data consisted of aggregated information on the physical quantities of inputs and outputs per ton of WB chemical (fermentable sugar, auxiliaries and final energy use by types) as well as total investment costs and labor requirements. For PDO and lactic acid, industry data stemmed from industrial plants of DuPont (*45*) and NatureWorks (*46*). For ethanol, lysine, and succinic acid, it originated from pilot plants (*10,32,47*). These data are referred to as industry data.

Prices of Fermentable Sugars

Fermentable sugar was the feedstock of WB processes and its price influenced the economics of WB products. Fermentable sugar may be raw or refined and consists of biomass-derived readily fermentable carbohydrates such as sucrose, hydrolyzed starches, or pretreated and hydrolyzed lignocellulose, which is still an emerging technology. In order to account for variations in fermentable sugar prices both in the near and longer-term future and for world regions, calculations were carried out for four price levels of fermentable sugar. The lowest price of $70 \notin/t$ represents local sugar prices in Brazil*: due to good climatic conditions and the availability of very cheap labor, the production cost of fermentable sugar from sugar cane was at its lower boundary. The high sugar price of $200 \notin/t$ represents a 10-yr average of world raw sugar (contract 11) as traded at the New York

^{*}Based on an average sugar price of R\$200 for the 2003/2004 season (48) and an exchange rate of 1 R = $0.29 \in$ for the same time frame.

Board of Trade (49). An intermediate price was chosen at $135 \notin/t$. An extreme level at $400 \notin/t$ represents a 10-yr average of US domestic raw sugar (contract 14) as traded at the New York Board of Trade (50). These price levels were based on raw sugar prices. However, if the micro-organism is sensitive to impurities then refined sugar will be used for fermentation. World refined sugar as traded at the London Stock Exchange has been traded for an average price of ca. $250 \notin/t$ during the last 10 yr (51) and thus within the range of prices considered. The price ranges for a ton of fermentable sugar were exogenous inputs to our calculations, i.e., we do not perform economic analyses for different combinations of feedstock types with technologies for producing fermentable sugar.

Petrochemical Process Data

In this paper we differentiate between WB industry data (*see* "WB Industrial Process Data") and petrochemical data. With petrochemical data we mean PCPP values of bulk petrochemicals which have been calculated according to the method described in "Process Economics Methodology." The required process data on inputs, outputs, labor requirements and investment costs stems from SRI (52). Prices of petrochemical products were based on a crude oil price of US \$25 per barrel, but a sensitivity analysis was carried out with twice this price (*see* "Sensitivity Analysis for High Crude Oil Prices").

Although petrochemical process technologies may improve in the future, we did not take into account any technological progress and always used current petrochemical technology for comparisons (*see* "Sensitivity to Key Technical Parameters" for a discussion). Typical plant sizes range between 50 kt/yr for maleic anhydride and 700 kt/yr for ethylene and acetic acid. We kept plant sizes larger than 100 kt/yr unchanged but increased production capacities of premarket products such as PDO and PTT to 100 kt/yr if they were smaller (*52*), using scaling factors of 0.75 for investment costs and 0.25 for labor.

Similar to WB products, petrochemical products may also show discrepancies between market prices and PCPPs. By analogy to the explanation given in "Process Economics Methodology," the PCPP of a petrochemical product is usually substantially lower than its market price if the product is new on the market and/or if it is used for niche applications. If the PCPP of the petrochemical product is higher than the market price this is typically the consequence of fierce competition accompanied by overcapacities. The difference between the market price and the PCPP can be substantial for both WB and petrochemical products. Because this difference was largely unpredictable, we based our economic comparisons for current and future technology on the PCPPs of the WB products and their petrochemical counterparts to ensure a level playing field.*

^{*}Market prices of petrochemicals may be used if the distorted situation is expected to continue or if a "snapshot" of the current situation is required.

Prices of Utilities and Auxiliaries

For the economic assessment, we assume a default stock market crude oil price of US \$25 per barrel (bbl; $4.1 \notin/GJ$) and a natural gas price of $4 \notin/GJ$. Prices were valid for the year 2000 for large West European industry. This corresponds to an estimated electricity price of $15 \notin/GJ_e$ and a steam price of $12 \notin/t$ ($5.7 \notin/GJ$). The sensitivity analysis in "Sensitivity Analysis for High Crude Oil Prices" studies the effect of higher energy prices, with a crude oil price of US \$50/bbl ($8.2 \notin/GJ$), a natural gas price of $6 \notin/GJ$, and corresponding steam and power prices of $17 \notin/t$ ($8.3 \notin/GJ$) and $16 \notin/GJ_e$ respectively. Economic credits were introduced in order to account for the avoided production of heat and power in case energy was recovered.

Enzyme and membrane prices were assumed to decrease in the future as a result of their large-scale production. Enzyme prices for current technology were set to $100 \notin$ /kg and were assumed to decrease by a factor of 10 for future technology, the prices of high-quality membranes were set to $100 \notin$ /ton of product and were assumed to decrease by a factor of two.

Case Study on 1,3-Propanediol

In order to provide insight into the type of analysis performed, this section presents the findings of the techno-economic assessment in a detailed case study on PDO. PDO is used to produce PTT, a polymer with the potential to replace nylon and PET fibers. We select PDO for this case study because both the petrochemical and the WB-based routes are currently being pursued by industry: Shell currently produces PDO from petrochemical feedstocks, whereas DuPont is building a plant for PDO production based on fermentable sugars from maize starch. The same type of analysis was performed for the other products, the results of which will be presented in condensed form in "Results."

Production Routes

Four different production routes of WB-based PDO were calculated according to the generic approach and were then compared to industry data on the production of PDO by means of WB as well as petrochemistry. The four WB routes studied with the generic approach all consist of aerobic fermentation of fermentable sugar* to PDO, with seed train, inoculum train, fermentation, and ultrafiltration steps, followed by different types of downstream processing. Routes 1 and 2 represent current technology, with downstream processing by distillation. Routes 3 and 4 represent future technology, where separation of PDO occurs by pervaporation, which has been successful on the laboratory scale (53). DuPont's route consists of aerobic fermentation with undisclosed downstream processing. The petrochemical route results in PDO via hydroformylation of ethylene oxide.

^{*}Routes based on glycerol as a feedstock are calculated in ref. 2, but are found to be significantly more expensive than the routes presented here.

Technology fermen downstream proces	tation	<i>Route 1</i> <i>Today</i> Batch distillation	<i>Route 2</i> <i>Today</i> Continuous distillation	<i>Route 3</i> <i>Future</i> Continuous pervaporation of water	<i>Route 4</i> <i>Future</i> Continuous pervaporation of PDO
Inputs	unit				
Dextrose	t	2.4	2.4	1.9	1.9
Nutrients	t	0.1	0.1	0.1	0.1
Process water	t	0.7	0.7	0.7	0.7
Electricity	GJ	9.1	2.9	1.6	1.4
Steam	t	6.6	6.6	10.2	0.9
Membranes	€	50.0	50.0		
Outputs					
PDO	t	1.0	1.0	1.0	1.0
Waste biomass	t	0.2	0.2	0.1	0.1
Fixed costs					
ISBL ^a	M€	75	67	42	39
$OSBL^{a}$	M€	28	25	20	18
Labor ^a	fte	28	15	11	11

Table 5 Process Inputs and Outputs for the Production of 1 Ton of 1,3-Propanediol (PDO) (at the Plant Gate) With Current and Future Technology as well as Related Investment Costs and Labor Requirements for a 100-kt Plant

^{*a*}Costs for inside battery limits (ISBL) outside battery limits (OSBL) and labor are given for an entire plant, based on a capacity of 100 kt. ISBL deals with the core process equipment, piping, instrumentation, etc. OSBL deals with steam and power generation and supply, wastewater treatment, cooling towers, etc. "Fte" is short for full time equivalents..

Based on the data for concentrations, productivities, and yields from Table 2, mass and energy balances were established. The energy balance was derived from energy requirements of unit processes (*see* Table 4). Table 5 shows the resulting in- and outputs for the four WB routes according to the generic approach.

Results for PDO Production Routes

Following the methodology, the inputs and outputs according to the generic approach as well as from industry and petrochemical process data were used to calculate the PCPP of the different routes to PDO. Figure 3 shows the resulting PCPPs for routes 1 and 4 according to the generic approach, for DuPont's WB route, and for the petrochemical pathway as well as the current market price of PDO. The values for routes 2 and 3 remain between those of routes 1 and 4 (*see also* Fig. 4).

The PCPP values of route 1 and industry coincide well, thereby corroborating the generic approach. As shown in Fig. 3, substantial savings are possible with current state-of-the-art technology relative to the market price. However, PDO is a relatively new product that is currently manufactured in small quantities and sold at high prices for niche applications.



Fig. 3. 1,3-propanediol (PDO) production cost plus profits (PCPP) for today's and future white biotechnology processes compared to both petrochemical PCPP and current market price for PDO (energy price level: US\$25/bbl).



Fig. 4. Cost composition for 1,3-propanediol (PDO) production for the industry and 4 generic production routes of PDO for low (70 \in /t) and high (400 \in /t) prices of fermentable sugar (crude oil price: US \$25/bbl) as well as the petrochemical production route for crude oil prices of US \$25/bbl and US \$50/bbl.

Instead of using the current market price as a benchmark, it was therefore better to choose the PCPP of petrochemical PDO. This comparison shows that for future technology (route 4), PDO is competitive with petrochemical PDO for a sugar price of up to 400 €/t and crude oil prices of US \$25/bbl.

Composition of Production Costs

In order to better understand the main factors determining the PCPP, we discuss the contribution of feedstock costs, utility costs, capital charge, and the remainder (other costs). Feedstock costs depend on both the amount of fermentable sugar required and its price level. Utility costs can differ considerably between current and future technology. The investment costs depend on the number of fermentation vessels needed (determined by the productivity level) and the type of downstream processing, e.g., the number of extraction columns.

Figure 4 shows that for high fermentable sugar prices $(400 \notin /t)$, feedstock costs alone may be higher than the total PCPP for low sugar prices $(70 \notin /t)$. For low and medium sugar prices, dependence on feedstock prices of WB-based PDO was much weaker compared to petrochemical PDO.* For very high sugar prices, the contribution of feedstock costs was higher for WB processes compared to the petrochemical processes. Finally, a doubling of the oil price leads to feedstock costs that are almost equal to the PCPP of the low oil price.

Results

PCPPs were calculated for all WB products using the methodology described above (*see* Fig. 2). Table 6 shows the results not only for the generic approach (*see* rows labeled "Today" and "Future") but also for industry data. For lactic acid, acrylic acid, and caprolactam, no generic approach calculations were available for today's technology (*see* "Technology Assumptions for WB Routes"). The ranges specify PCPPs of at least two different separation processes (*see* Table 3) in the generic approach or different datasets in the case of industry data and show the whole range of PCPPs calculated. The petrochemical PCPPs in Table 6 refer to benchmark substances that are chemically identical with the bio-based compounds, unless indicated otherwise. In the cases of lactic acid and lysine, no petrochemical benchmarks can be given because these products are produced from bio-based feedstocks via WB already today; in these cases the comparison was made with current industrial practice.

Comparing the results of the generic approach for today's technology to industry data (for those products where both were available), we conclude that the results correlate well for lysine, PDO, and PTT, where the PCPPs are in the same range. In the case of succinic acid, the calculations according to the generic approach are somewhat lower than the industry

^{*}Note that there is a methodological difference between the two petrochemical PDO cases: whereas the first case (crude oil price of US\$25/bbl) uses market prices for the inputs to production, the second case uses PCPPs for these inputs, because market prices at a crude oil price of US\$50/bbl were not available (*see also* "Sensitivity Analysis for High Crude Oil Prices").

Pro	oduction Cost Pl and Future Tecl s Well as Indust	lus Profits (€/t) hnology Accor ry, of the Ptroc) of White Biot ding to the Ger hemical Bench	Table 6 echnology Prod neric Approach mark and the M	lucts for Varyii (Rows Entitlec Aarket Price (fo	ng Sugar Prices an 1 "Today" and "Fu or US \$25/barrel ci	id Current uture″) rude oil)
			Product	tion cost plus p	rofits (€/t)		
		Bio-based	as a function o	f fermentable sı	ıgar price		
Product	Technology	70 €/t	135 €/t	200 €/t	400 €/t	Petrochemical	Market price (€/t)
ABE	Today	1160–1230	1370 - 1430	1570 - 1640	2210-2270	700	500
	Future	390 - 480	570 - 660	740 - 830	1270 - 1360	n-buta	anol
Acetic acid	Today	2070–2080	2210-2220	2350–2360	2770–2790	370	400
	Future	620-750	700-820	780–900	1020 - 1140		
Acrylic	Future	960	1050	1150	1440	1050	880
Adipic acid	Today	2580	2980	3380	4600	1100	1090
I	Future	980-1050	1120 - 1200	1270 - 1350	1720 - 1810		
Ethanol	Industry	510	660	800	1260	870	440
	Today	500 - 570	650-730	800 - 880	1260 - 1350		
	Future	360–370	510 - 520	660–670	1110-1130		
Lactic acid	Industry	006-069	770–980	850 - 1060	1090 - 1300	I	1390
	Future	390 - 410	460 - 485	540 - 560	770-800		
$Lysine^{a}$	Industry	1230–2110	1450 - 2300	1670 - 2490	2350–3080	I	1440
	Today	1580	1890	2200	3160		
	Future	810	1030	1250	1920		
PDO	Industry	096-006	1050 - 1070	1190 - 1210	1550–1690	1120	2410
	Today	660-820	830–990	1000 - 1160	1510–1670		
	Future	470–600	600-730	730–860	1130–1260		
PHA	Today	1090 - 2220	1310 - 2430	1530 - 2640	2220–3280	930	1100
	Future	1090	1250	1420	1930	PE	

Succinic acid	Industry	1110	1180	1250	1460	860	700
	Today	750-870	830–950	910-1020	1150 - 1260	Maleic anh	ydride
	Future	470 - 570	540 - 640	610-710	820-920		
Caprolactam	Future	1200	1380	1560	2100	1860	1320
Ethyl lactate	Today	1090	1220	1350	1750	860	650
ı	Future	790-890	920-1020	1040 - 1140	1420 - 1530	Ethyl ace	tate
Ethylene	Today	1050	1320	1590	2430	610	720
	Future	820	1080	1340	2140		
PLA	Industry	1310 - 1420	1410 - 1520	1510 - 1630	1830 - 1940	1050	1200
	Future	1180 - 1280	1270 - 1380	1370 - 1480	1670 - 1770	PET	
PTT	Industry	1090 - 1110	1150 - 1160	1200 - 1210	1340 - 1400	1180	
	Today	1000 - 1060	1060 - 1130	1130 - 1190	1330 - 1390		
	Future	750	750	750	760		
^{<i>a</i>} Lysine can b	e produced and s	old as a salt conta	uining different ic	ons and in varying	g degrees of purity,	costs are therefore	standardized for 1 ton

lysine content.
ABE, acetone-butanol-ethanol; PDO, 1,3-propanediol; PHA, polyhydroxyalkanoates; PLA, polylactic acid; PTT, polytrimethylene terephtha-
late.



Fig. 5. Economic viability of today's white biotechnology technology: ratio of production cost plus profits (PCPP) of the WB product to its petrochemical counterpart for today's technology as a function of the sugar price level (for 25US\$/barrel crude oil)

data: investment costs for downstream processing are higher for the latter. In general, the PCPPs of current technology according to the generic approach and those of industry are in the same range, with a small spread of 5–10% for a given price of fermentable sugar. An exception is the large spread in industry data on lysine, which is due to differences in salt composition and degrees of purity. We therefore conclude that the generic approach yields reliable results.

Most importantly, Table 6 shows that for current technology, 30% of WB products are economically viable for low sugar prices. PDO, PTT, and ethanol are economically viable even for high sugar prices ($200 \notin /t$). These findings are more directly visible from Fig. 5, which shows the ratio of PCPPs of the current technology WB products compared to their petrochemical counterparts. Values below 100% indicate that the production costs are lower for the WB product, whereas values above 100% represent cases in which the production of the WB product is more expensive than its petrochemical counterpart. The PCPP ratio of acetic acid ranges from 550% to 740% and therefore lies outside of the range of Fig. 5.

By analogy, Fig. 6 shows the ratios of PCPP for future technology WB products to the (current technology) petrochemical. Almost all products researched offer economic savings for a sugar price of $70 \notin /t$, with the exception of acetic acid, ethylene, and PLA.

In conclusion, technological progress can contribute significantly to improve economic viability of WB products: on average, the PCPPs of products that are directly obtainable from fermentation (e.g., lactic acid) are 40– 50% lower than for today's technology; for products that require a chemical conversion after fermentation (e.g., PLA), technological progress reduces

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Fig. 6. Economic viability of future white biotechnology (WB) technology: ratio of production cost plus profits (PCPP) of the WB product compared to its petrochemical counterpart for future technology as a function of the sugar price (for 25 \$US/barrel crude oil).

Table 7
Viability of White Biotechnology (WB) Chemicals for Four Price Levels
of Fermentable Sugar for Current and Future Technology
(crude oil price: US \$25/bbl)

Sugar price	Today	Future
400 €/t 200 €/t	PDO (possibly) PDO, PTT, ethanol	Lactic acid, PTT, lysine, PDO (possibly) Lactic acid, PTT, lysine, PDO, caprolactam, ethanol, succinic acid
135 €/t	PDO, PTT, ethanol	Lactic acid, PTT, lysine, PDO, caprolactam, ethanol, succinic acid, ABE
70 €/t	PDO, PTT, ethanol, succinic acid, PHA (possibly)	Lactic acid, PTT, lysine, PDO, caprolactam, ethanol, succinic acid, ABE, acrylic acid, adipic acid, ethyl lactate, PHA (possibly), PLA (possibly)

"Possibly" indicates that the production cost plus profits (PCPP) of the WB chemical is higher than the PCPP of its petrochemical equivalent, but lower than the current market price of the product. PDO, 1,3-propanediol; PTT, polytrimethylene terephthalate; PHA, polyhydroxyalkanoates; PLA, polylactic acid; ABE, acetone-butanol-ethanol.

the PCPP by approx 20%. This results in many more products becoming economically viable in the future, even at rather high sugar prices. Table 7 summarizes the viability of current and future WB chemicals for four sugar prices.

Discussion

Sensitivity Analysis for High Crude Oil Prices

This sensitivity analysis investigates the effect of the crude oil price on the competitiveness of the WB products compared to their petrochemical counterparts. The crude oil price is set to US $50/bbl (8.9 \in/GJ)$ and the natural gas price* for end users to $6 \in/GJ$. Our analysis accounts for increased prices of feedstock and auxiliaries as well as utilities but not for increased investment costs as a consequence of higher energy costs.

In order to perform the calculations for a crude oil price of US \$50/bbl, the methodology has to be adapted: whereas for the default case (US \$25/bbl), we use market prices for feedstocks and auxiliaries, these are not available to us for an oil price level of US \$50/bbl. For this reason, we use PCPPs for these process inputs instead of market prices. In the cases of ethyl acetate and PET, some petrochemical process inputs have higher PCPPs than market prices even for the low crude oil price (US \$25/bbl), leading to PCPP values that are significantly higher (by 30–70%) than those presented in Table 6. This indicates that their production is not economically viable. For all other products and their petrochemical counterparts, the PCPPs derived from this changed method differ only to a small extent (by 4% on average) from the PCPPs presented earlier.

The sensitivity analysis is performed for a selection of WB-based products that have a high chance of gaining a large market share, i.e., ABE, acetic acid, adipic acid, ethanol, ethyl lactate, ethylene, PDO, PHA, PLA, PTT, and succinic acid (we therefore exclude acrylic acid, caprolactam, lactic acid, and lysine). In general, the PCPPs of the petrochemical products are found to increase by 23% on average as a result of higher feedstock and energy costs, whereas the PCPPs of the WB products only increase by 4–6% because of higher utility costs. Some WB products become economically competitive even at the highest sugar price, both with current and future technology, for example PDO, PTT, and succinic acid. The values for acetic acid are outside the range of Fig. 7 (the economic viability deteriorates compared to lower crude oil prices as a result of the large amount of energy necessary in downstream processing).

In the case of future technology ethylene, the WB product is economically competitive with the petrochemical product for the high crude oil price (US \$50/bbl) up to a sugar price of 135 €/t. For PLA, the effect of higher oil and gas prices is even larger: it is economically viable for the high crude oil price (US \$50/bbl) up to the highest sugar price for future technology. On average, relative economic viability^[1] of WB products increases by 25% (ethylene is an exception and increases by 70%). This indicates that

^[1](PCPP_{WB} / PCPP_{petrochemical})_{US \$25/bbl} / (PCPP_{WB} / PCPP_{petrochemical})_{US \$50/bbl}

^{*}The natural gas price for the high crude oil price is calculated based on a factor of 1.5 for a doubling of the oil price, corresponding to the IPCC SRES B1 and B2 scenarios (54).





the development of the oil price will have a significant effect on the economic viability of WB products. Comparing Figs. 5 and 6 to Fig. 7 it becomes clear that at the higher oil price more WB products have a PCPP ratio of less than 100%, i.e., are economically viable. A more detailed scenario analysis dealing with a larger variety of oil prices for a selection of products is carried out by Dornburg (*18*).

Sensitivity to Economic Parameters

All WB calculation results presented refer to a plant capacity of 100 kt per year, but for most of the products studied, sensitivity analyses have been performed for larger plant sizes (200 kt to 400 kt per year) for future technology. The results of the sensitivity analysis show that larger scale production plants reduce the PCPP of the WB routes by on average 10% (range: 5–20%) for a high sugar price of $400 \notin /t$ and 16% (range: 10–30%) for a low sugar price of $70 \notin /t$.

A sensitivity analysis was also carried out for a lower capital charge of 10% of the TFC instead of 30% for current and future technology. This reduced the PCPP on average by 15% (range: 5–25%) for the high sugar price of $400 \notin/t$ and by 25% (range: 10–35%)Y for the low sugar price of $70\notin/t$. The average sensitivities of the petrochemical equivalents are 20% both to scale* and to capital charge. Therefore, both scale and capital charge are found not to significantly influence the economic competitiveness of the WB product compared to the petrochemical equivalent. The results are therefore rather robust both to scale and capital charge.

Sensitivity to Key Technical Parameters

To quantify the effect of improved biotechnology, data on production of electricity, fertilizer, and biomass yields in agriculture were kept constant throughout the analysis. However, it is likely that these technologies will also improve in the future. For all comparisons, current technology was assumed for petrochemical production routes: it has not been taken into account that petrochemical processes will also improve in the future. Including technological progress in petrochemical processes would lead to smaller benefits by WB because savings in process energy of 20% and beyond are possible for future technology petrochemicals (*55*). However, utilities only make up 3% of the PCPP of petrochemical ethylene, and savings in the range of 20% will therefore not significantly change the relative PCPPs of WB chemicals compared with petrochemicals.

Additionally, the economic calculations of future WB technology routes strongly rely on the key assumptions on productivities, yields and concentrations (Table 2). The values assumed for these key parameters were critically reviewed by project partners and are considered to repre-

^{*}Sensitivity to scale implies downscaling to 100 kt/yr in most cases, since petrochemical plant sizes larger than 100 kt/yr were kept unchanged (*see* "Petrochemical Process Data").

sent the technical potential that may be reached after two to three decades of R&D. A sensitivity analysis is performed for future ethanol production to assess the influence of the values assumed for future productivity: a significantly lower productivity of $10 g/(L\cdot h)$ instead of $50 g/(L\cdot h)$ increases the PCPP only by 5% for the whole range of sugar prices. In general, the real technical data are expected to remain below the values in Table 2 within the next 10 yr and the real economic viability for this timeframe may therefore fall short of our calculations. More details of the sensitivity analyses are also available in ref. 2.

Comparison With Earlier Publications

Production of succinic acid from maize starch (15) and glucose (16) results in succinic acid prices in ranges of US \$550-2200/t. These values are in line with the PCPPs from the generic approach (760–920 €/t for current technology). Production of ethanol from maize starch (12) and lignocellulosics (11) results in ethanol prices in the range of US \$650–960/t. These values correlate well with the PCPPs from the generic approach (500–1350 \in /t for current technology). Production of ABE from maize starch (14) results in butanol prices in the range of US \$340-1070/t. These values differ from the PCPPs from the generic approach (1170–2270 \in /t for current technology). There are three factors contributing to this difference: the price of maize, the choice of location and the credits from by-products. The price of (whole) maize is set to US \$79/t and US \$197/t, which translates into US \$56/t glucose and US \$140/t glucose.* Both values are at the lower end of the sugar prices used here. The type of plant has a significant influence; Qureshi and Blaschek (14) assume that the plant will be built as an extension to an existing corn milling plant, with proportionately lower investment costs compared to a grassroots plant as assumed in the generic approach. The credits from by-products are decisive: in this research, we only consider economic credits for acetone and ethanol produced, but not for gases, cell mass, remaining sugars, etc. The credits for acetone and ethanol only make up 17% of the by-product credits in ref. 14, with total by-product credits much larger than the revenues from butanol. Recalculating their data for a new plant, with by-product credits only for acetone and butanol, results in a butanol price of US \$1319/t (for a maize price of US \$197/t), well within the range of our results.

Comparison With Current Developments in Industry

The results from the generic approach show that the production of PDO/PTT is economically viable at the low crude oil price (US \$25/bbl). This is in line with current developments in industry, which show DuPont building a plant in Tennessee to produce bio-based PDO using fermentable

^{*}This is a rough calculation based on a conversion of 5.14 kg of maize into 3.65 kg of glucose and disregarding capital and labor requirements for the process.

sugars from maize. The generic approach also shows that bio-based ethanol is economically viable using current technology but although it is produced on a large scale for fuel use, it has not entered the chemical industry sector in West Europe. This may be due to the presence of already depreciated plants that continue to be used. Although the generic approach shows that PLA is not economically viable at the low crude oil price (US \$25/bbl), calculations for the high crude oil price (US \$50/bbl) show that PLA is viable for current technology up to a sugar price of 200 €/t and all sugar prices for future technology. High crude oil prices in recent years have validated NatureWorks' building of a large industrial PLA plant in Nebraska with production running since 2001. The results from the generic approach show that the production of PHA is economically viable at the high crude oil price (US \$50/bbl) for low and medium sugar prices. This is in line with current developments in industry, which show Archer Daniels Midland and Metabolix announcing plans to build a plant in Iowa to produce biobased PHA from maize starch (56).

Conclusions

In this paper we presented and applied a generic approach that allows the systematic evaluation of present and future production routes of biobased chemicals from WB, based on available data and consistent assumptions on future (bio)technology developments. The production costs plus profits of current technology according to the generic approach and those of industry are in the same range, implying that the generic approach yields reliable results.

In general, a large number of WB chemicals are economically viable compared to their petrochemical equivalents. This economic competitiveness depends to a large extent on the prices of oil and sugar. For a crude oil price of US \$25/bbl the following products are economically viable for current technology: 1,3-propanediol, polytrimethylene terephthalate (PPT), succinic acid and ethanol. Comparing current to future technology, production cost plus profits of products directly obtained from the fermentation step are 40–50% lower and 20% lower for products that require a chemical conversion step after fermentation for a crude oil price of US \$25/bbl and across all sugar prices. This shows that technological progress can contribute significantly to improved economic viability of white biotechnology chemicals.

For future technology, all studied products except for acetic acid, PLA, and ethylene are economically viable at fermentable sugar prices of $70 \in /t$. The sensitivity analysis shows that at a crude oil price of US \$50 per barrel, future technology ethylene will be economically viable for a sugar price of up to $135 \in /t$ and polylactic acid will be viable up to the highest sugar price. All other products improve in economic competitiveness.

A large-scale introduction of WB-based production of economically viable bulk chemicals would therefore be desirable if the environmental impacts are smaller than those of current petrochemical production routes (this is discussed in ref. 19). Under these conditions, white biotechnology could become the center of attention for the chemical industry as well as for policy-makers.

Acknowledgments

This research was partly supported by the European Commission (Research Directorate General), 5th Framework European Network (GROWTH) Program, by support of the project "BREW" with the full title "Medium and long-term opportunities and risks of the biotechnological production of bulk chemicals from renewable resources" (Contract No. G5MA-CT-2002-00014). We would like to thank the BREW project partners Agrotechnology and Food Innovations (A&F), BP Chemicals, Degussa, DSM Research, DuPont, NatureWorks, Novozymes, Roquette Frères, Shell International Chemicals and Uniqema who provided valuable input for the generic approach. We are particularly grateful to Dr. Tim Nisbet (Shell Chemicals) and to both Dr. Peter Nossin and Peter Simons (both DSM Research). We thank Manuela Crank for laying the foundation of large parts of this work and Morna Isaac for her contributions. The views expressed in this article are those of the authors.

References

- 1. EuropaBio (2005) Industrial or white biotechnology—a driver of sustainable growth in Europe, European Association for Bioindustries (EuropaBio), Brussels.
- 2. Patel, M., Crank, M., Dornburg, V., et al. 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, Utrecht University, Utrecht, Germany (2006).
- 3. Rogers, P. L. (2002) Australasian Biotechnology 12, 39–41.
- 4. Zanin, G. M., Santana, C. C., Bon, E. P. S., et al. (2000) Appl. Biochem. Biotech. 84, 1147–1162.
- Vink, E. T. H., Rábago, K. R., Glassner, D. A., and Gruber, P. R. (2003) *Polymer Degrad. Stab.* 80, 403–419.
- 6. EuropeanCommission (2003) in 2003/30/EC pp 5, Official Journal of the European Union.
- 7. Bachmann, R., Bastianelli, E., Riese, J., and Schlenzka, W. (2000) in *The McKinsey Quarterly*. pp. 92–99.
- Werpy, T. and Petersen, G. (2004) Top Value Added Chemicals from Biomass— Volume I—Results of Screening for Potential Candidates from Sugars and Synthesis Gas, NREL/TP-510-35523, National Renewable Energy Laboratory, Golden, CO.
- 9. EuropaBio (2003) White Biotech: a gateway to a more sustainable future, The European Association for Bioindustries (EuropaBio), Brussels.
- 10. SRI (2001) Chemicals from renewable resources, PEP 236, SRI Consulting, Menlo Park, USA.
- 11. Hamelinck, C. N., van Hooijdonk, G., and Faaij, A. P. C. (2005) *Biomass & Bioenergy* **28**, 384–410.
- 12. O'Brien, D.J., Roth, L.H., and McAloon, A.J. (2000) J. Membr. Sci. 166, 105-111.
- 13. Wooley, R., Ruth, M.F., Glassner, D.A., and Sheehan, J. (1999) Biotech. Progr. 15, 794-803.
- 14. Qureshi, N. and Blascheck, H. P. (2001) J. Ind. Microbiol. Biotechnol. 27, 292-297.
- 15. Zeikus, J. G., Jain, M. K., and Elankovan, P. (1999) Appl. Microbiol. Biotech. 51, 545–552.

- 16. Landucci, R., Goodman, B., and Wyman, C. E. (1994) Appl. Biochem. Biotech. 45/46, 677–696.
- 17. Lynd, L. R. and Wang, M. Q. (2004) J. Ind. Ecol. 7, 17-32.
- 18. Dornburg, V., Patel, M., and Hermann, B. G. (submitted) Scenario projections for future market potentials of bio-based bulk chemicals. *Environ. Sci. Tech.*
- 19. Hermann, B. G., Blok, K., and Patel, M. (submitted) Producing bio-based bulk chemicals using industrial biotechnology saves energy and combats climate change. *Environ. Sci. Tech.*
- 20. Wyman, C. E. (2003) Biotech. Progr. 19, 254–262.
- 21. Shih, I.-L., Shen, M.-H., and Van, Y.-T. (2006) Bioresource Technology 97, 1148–1159.
- 22. Weissermel, K. and Arpe, H.-J. (2003) *Industrial Organic Chemistry*, 4th ed. Wiley-VCH, Weinheim.
- 23. Glenz, W. (2004) in Kunststoffe. pp 76–78.
- 24. EU (2000) Competitiveness of the Chemical Industry Sector in the CEE Candidate Countries, Brussels.
- 25. Campos, E.J., Qureshi, N., and Blascheck, H. P. (2002) Appl. Biochem. Biotech. 99, 553–576.
- 26. Ezeji, T.C., Qureshi, N., and Blascheck, H.P. (2003) World J. Microbiol. Biotech. 19, 595–603.
- 27. Lee, Y.Y., Balasubramanian, N., and Kim, J.S. (2001) Appl. Biochem. Biotech. 92, 367–376.
- 28. Huang, Y. L., Mann, K., Novak, J. M., and Yang, S. T. (1998) Biotech. Progr. 14, 800–806.
- 29. Niu, W., Draths, K., and Frost, J. (2002) Biotech. Progr. 18, 201–211.
- 30. Gryta, M., Morawski, A. W., and Tomaszewska, M. (2000) Catalysis Today 56, 159–165.
- 31. Bayrock, D. and Ingledew, W. (2005) World J. Microbiol. Biotech. 21, 83-88.
- 32. SRI (2002) Biotechnology separation processes, PEP 188B, SRI Consulting, Menlo Park, USA.
- 33. SRI (1999) 1,3-propanediol and polytrimethylene terephthalate, PEP 227, SRI Consulting, Menlo Park, USA.
- 34. Akiyama, M., Tsuge, T., and Doi, Y. (2003) Polymer Degrad. Stab. 80, 183-194.
- 35. Lee, P. C., Lee, W. G., Lee, S. Y., Chang, H. N., and Chang, Y. K. (2000) *Biotech. Bioproc. Eng.* **5**, 379–381.
- 36. Reismann, H. B. (1988) Economic Analysis of Fermentation Processes. CRC Press, FL: p. 94.
- 37. Reddy Kunduru, M. and Pometto, A. L. (1996) J. Ind. Microbiol. Biotechnol. 16, 249-256.
- 38. Lee, J. H., Pagan, R., and Rogers, P. L. (1983) Biotech. Bioeng. 25, 659–669.
- 39. Wibowo, C., Chang, W.-C., and Ng, K. M. (2001) AIChE J. 47, 2474–2492.
- 40. Fidaleo, M. and Moresi, M. (2005) Biotech. Bioeng. 91, 556–568.
- 41. SRI (2002) Polyhydroxyalkanoates from organic wastes, PEP 2002–8, SRI Consulting, Menlo Park, USA.
- 42. Wisniewski, M. and Pierzchalska, M. (2005) J. Chem. Technol. Biotechnol. 80, 1425–1430.
- 43. Lee, K.-R., Teng, M.-Y., Lee, H.-H., and Lai, J.-Y. (2000) J. Membr. Sci. 164, 13–23.
- 44. Simons, P. and Nossin, P. (2005) personal communication.
- 45. Alles, C. (2003) personal communication.
- 46. Vink, E. T. H. (2005) personal communication.
- 47. SRI (1999) Lysine-Sulfate Production By Fermentation with Recovery by Spray Drying, PEP 97–8, SRI Consulting, Menlo Park, USA.
- 48. ORPLANA (2005) Sugarcane payment in the Sao Paulo state—in the 2003/04 season http://www.orplana.com.br/estatisticas.asp.
- 49. NYBOT (2005) Historical data—Sugar 11, http://www.nybot.com/reports historicalData/indexHistoricalData.htm.
- 50. NYBOT (2005) Historical data—Sugar 14, http://www.nybot.com/reports historicalData/indexHistoricalData.htm.
- 51. Rupp-Dahlem, C. (2005) personal communication.
- 52. SRI (2000) *PEP Yearbook International*, Vol. 2M—Germany, SRI Consulting, Menlo Park, USA.
- 53. Li, S., Tuan, V. A., Falconer, J. L., and Noble, R. D. (2001) J. Membr. Sci. 191, 53–59.
- 54. Nakicenovic, N., Alcamo, J., Davis, G., de Vries, B., Fenhann, J., et al. (2000) Special report on Emission Scenarios (SRES), 599 p, Cambridge University Press, Cambridge.
- 55. Ren, T., Patel, M., and Blok, K. (2006) Energy 31, 425–451.
- 56. ArcherDanielsMidland (2006) ADM Names Clinton, Iowa as Location for PHA Plant, http://www.admworld.com/naen/pressroom/.