

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

A Techno-Economic Analysis

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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 €/t and 400 €/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-by-product 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 dia-

gram 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^t 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).

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

| 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 |

^aThe 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.

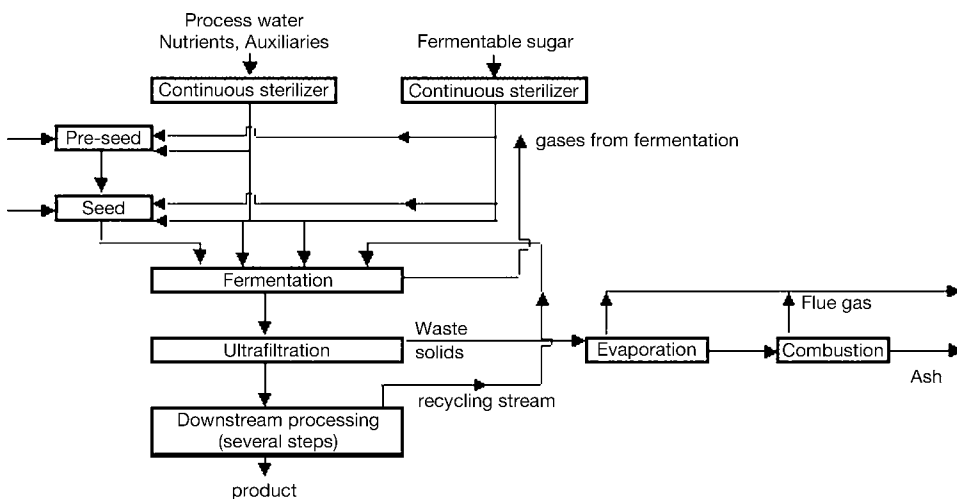


Fig. 1. Simplified flowsheet as used in the generic approach.

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·h]).

[‡]Yield is defined as the mass of the product divided by the mass of the fermentable sugar (in g/g)

Table 2
Type of Fermentation and Key Data on Concentration, Productivity, and Yields
of Fermentation for Current and Future Technology

| Product | Type of fermentation | | Broth concentration g/L | Productivity g/(L.h) | Yield g product/g glucose | Reference |
|------------------|----------------------|-----------------------|-------------------------|----------------------|---------------------------|-----------|
| | Today/ future | Aerobic/ anaerobic | | | | |
| 1 ABE (butanol) | Today | anaer. | 20 | 0.36 | 0.42 | 14,25,26 |
| | Future | anaer. | 45 | 15 | 0.50 | |
| 2 Acetic acid | Today | anaer. | 18 | 0.15 | 0.50 | 27,28 |
| | Future | anaer. | 50 | 15 | 0.90 | |
| 3 Acrylic acid | Future | anaer. | 50 | 10 | 0.72 | 29 |
| 4 Adipic acid | Today | aerobic | 20 | 0.42 | 0.17 | |
| 5 Ethanol | Future | aerobic | 40 | 10 | 0.47 | 17,30,31 |
| | Today | anaer. | 100 | 2.2 | 0.46 | |
| 6 Lactic acid | Future | anaer. | 130 | 50 | 0.47 | 32 |
| | Future | anaer. | 180 | 20 | 0.95 | |
| 7 Lysine | Today | aerobic | 100 | 1.7 | 0.34 | 33 |
| | Future | aerobic | 140 | 10 | 0.63 | |
| 8 PDO | Today | aerobic | 100 | 1.67 - 6 | 0.41 | 34 |
| | Future | aerobic | 100 | 15 | 0.54 | |
| 9 PHA | Today | aerobic | 150 | 3.0 | 0.35 | 10,35 |
| | Future | aerobic | 150 | 10 | 0.43 | |
| 10 Succinic acid | Today | anaer. | 80 | 1.8 | 0.88 | 10,35 |
| | Future | anaer. | 150 | 15 | 1.01 | |

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

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 CO₂ 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 CO₂ 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.

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

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

^aFor 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

Table 4
Key Data on Specific Energy Use of Unit Processes

| 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 |
| | 0.04 | kWh power/kg evaporated |
| Evaporation of water, multi-stage | | |
| | 0.5 | kg steam/kg evaporated |
| | 0.005 | kWh power /kg evaporated |
| Distillation | 1.3 * product's heat of evap. | kg steam/kg evaporated |

^aAn equivalent is here considered as the number of dissociation 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-feed-

stocks 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 €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 with a fixed percentage. In consultation with industry experts, a 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.

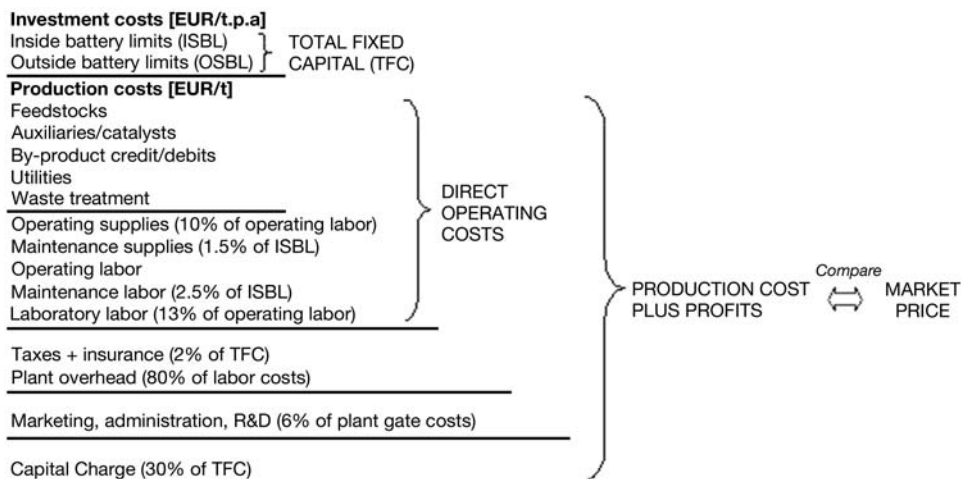


Fig. 2. Procedure to calculate production costs plus profits (PCPP).

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 €/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 €/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 € for the same time frame.

Board of Trade (49). An intermediate price was chosen at 135 €/t. An extreme level at 400 €/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 €/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 €/GJ) and a natural gas price of 4 €/GJ. Prices were valid for the year 2000 for large West European industry. This corresponds to an estimated electricity price of 15 €/GJ_e and a steam price of 12€/t (5.7 €/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 €/GJ), a natural gas price of 6 €/GJ, and corresponding steam and power prices of 17 €/t (8.3 €/GJ) and 16 €/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 €/kg and were assumed to decrease by a factor of 10 for future technology, the prices of high-quality membranes were set to 100 €/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.

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

| | | Route 1 | Route 2 | Route 3 | Route 4 |
|-------------------------|-----------------|--------------|--------------|---------------------------|-------------------------|
| | | Today | Today | Future | Future |
| Technology fermentation | | Batch | Continuous | Continuous | Continuous |
| downstream processing | | distillation | distillation | pervaporation of water | pervaporation of PDO |
| <i>Inputs</i> | | | | | |
| | 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 _e | 9.1 | 2.9 | 1.6 | 1.4 |
| Steam | t | 6.6 | 6.6 | 10.2 | 0.9 |
| Membranes | € | 50.0 | 50.0 | | |
| <i>Outputs</i> | | | | | |
| PDO | t | 1.0 | 1.0 | 1.0 | 1.0 |
| Waste biomass | t | 0.2 | 0.2 | 0.1 | 0.1 |
| <i>Fixed costs</i> | | | | | |
| ISBL ^a | M € | 75 | 67 | 42 | 39 |
| OSBL ^a | M € | 28 | 25 | 20 | 18 |
| Labor ^a | fte | 28 | 15 | 11 | 11 |

^aCosts 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.

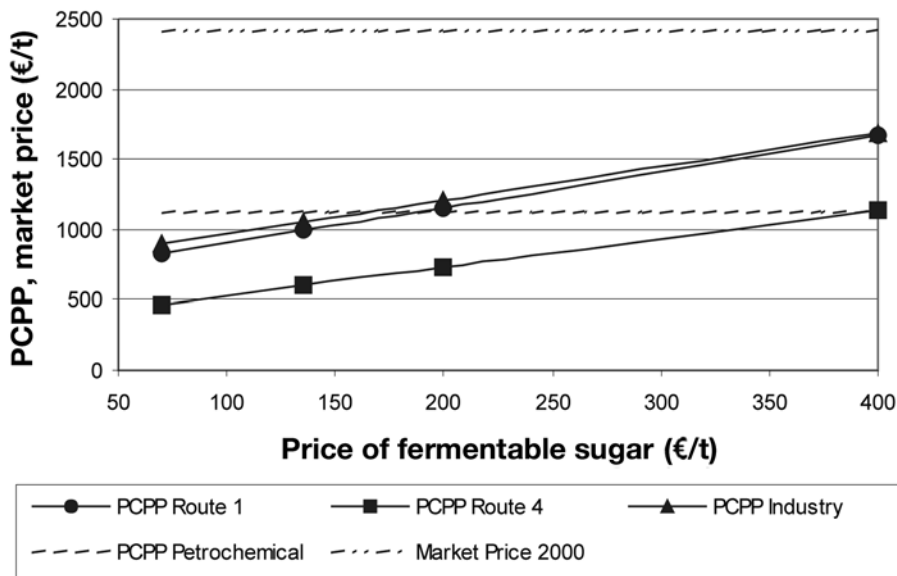


Fig. 3. 1,3-propanediol (PDO) production cost plus profits (PCPP) for today's and future white biotechnology processes compared to both petrochemical PCPP and current market price for PDO (energy price level: US\$25/bbl).

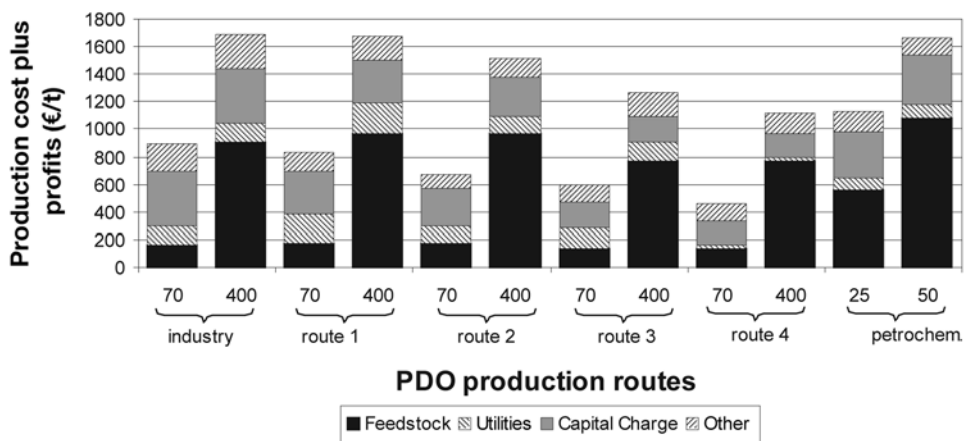


Fig. 4. Cost composition for 1,3-propanediol (PDO) production for the industry and 4 generic production routes of PDO for low (70 €/t) and high (400 €/t) prices of fermentable sugar (crude oil price: US \$25/bbl) as well as the petrochemical production route for crude oil prices of US \$25/bbl and US \$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 €/t), feedstock costs alone may be higher than the total PCPP for low sugar prices (70 €/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").

Table 6

Production Cost Plus Profits (€/t) of White Biotechnology Products for Varying Sugar Prices and Current and Future Technology According to the Generic Approach (Rows Entitled "Today" and "Future") as Well as Industry, of the Petrochemical Benchmark and the Market Price (for US \$25/barrel crude oil)

| Product | Technology | Production cost plus profits (€/t) | | | | | | | Petrochemical | Market price (€/t) |
|---------------------------|------------|--|-----------|-----------|-----------|--------------------|---------|---------------|---------------|--------------------|
| | | Bio-based as a function of fermentable sugar price | | | | | 400 €/t | Petrochemical | | |
| | | 70 €/t | 135 €/t | 200 €/t | 400 €/t | 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-butanol | | | | |
| 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 | | | |
| | 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 | | | | | |
| Lactic acid | Future | 360-370 | 510-520 | 660-670 | 1110-1130 | — | 1390 | | | |
| | Industry | 690-900 | 770-980 | 850-1060 | 1090-1300 | | | | | |
| Lysine^a | Future | 390-410 | 460-485 | 540-560 | 770-800 | — | 1440 | | | |
| | Industry | 1230-2110 | 1450-2300 | 1670-2490 | 2350-3080 | | | | | |
| PDO | Today | 1580 | 1890 | 2200 | 3160 | | | | | |
| | Future | 810 | 1030 | 1250 | 1920 | | | | | |
| PHA | Industry | 900-960 | 1050-1070 | 1190-1210 | 1550-1690 | 1120 | 2410 | | | |
| | Today | 660-820 | 830-990 | 1000-1160 | 1510-1670 | | | | | |
| PE | Future | 470-600 | 600-730 | 730-860 | 1130-1260 | 930 | 1100 | | | |
| | Today | 1090-2220 | 1310-2430 | 1530-2640 | 2220-3280 | | | | | |
| PE | Future | 1090 | 1250 | 1420 | 1930 | | | | | |

| | | | | | | | |
|----------------------|----------|-----------|-----------|-----------|-----------|------------------|------|
| Succinic acid | Industry | 1110 | 1180 | 1250 | 1460 | 860 | 700 |
| | Today | 750-870 | 830-950 | 910-1020 | 1150-1260 | Maleic anhydride | |
| Caprolactam | Future | 470-570 | 540-640 | 610-710 | 820-920 | | |
| | Future | 1200 | 1380 | 1560 | 2100 | 1860 | 1320 |
| Ethyl lactate | Today | 1090 | 1220 | 1350 | 1750 | 860 | 650 |
| | Future | 790-890 | 920-1020 | 1040-1140 | 1420-1530 | Ethyl acetate | |
| 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 | | |

^aLysine can be produced and sold as a salt containing different ions and in varying 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 terephthalate.

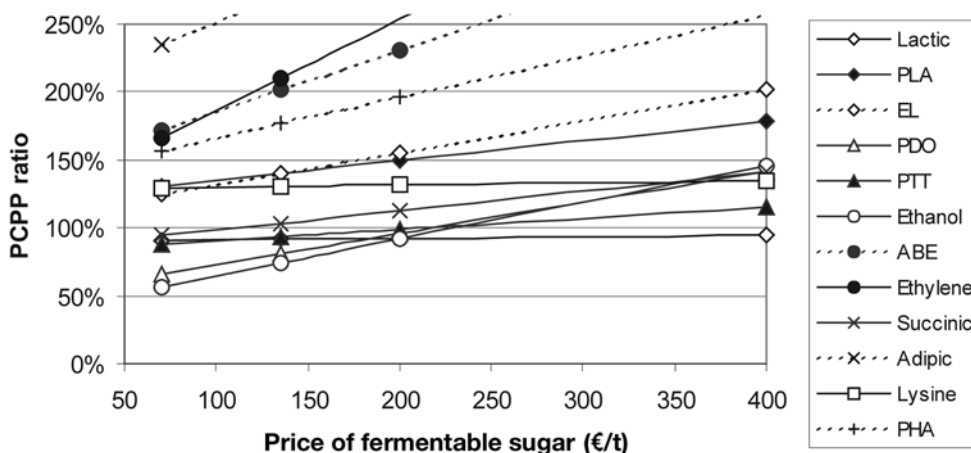


Fig. 5. Economic viability of today's white biotechnology technology: ratio of production cost plus profits (PCPP) of the WB product to its petrochemical counterpart for today's technology as a function of the sugar price level (for 25US\$/barrel crude oil)

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 €/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 €/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

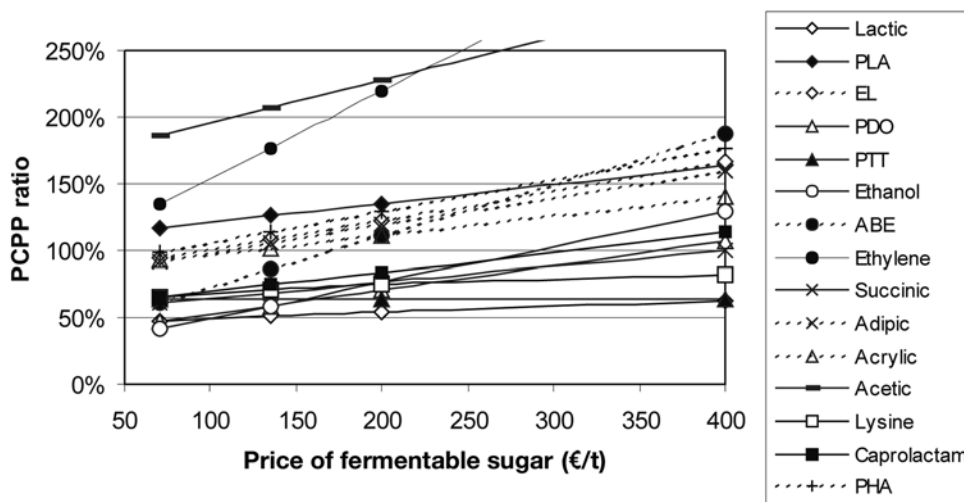


Fig. 6. Economic viability of future white biotechnology (WB) technology: ratio of production cost plus profits (PCPP) of the WB product compared to its petrochemical counterpart for future technology as a function of the sugar price (for 25 \$US/barrel crude oil).

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 | PDO (possibly) | Lactic acid, PTT, lysine, PDO (possibly) |
| 200 €/t | PDO, PTT, ethanol | 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 €/GJ) and the natural gas price* for end users to 6 €/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] $(\text{PCPP}_{\text{WB}} / \text{PCPP}_{\text{petrochemical}})_{\text{US } \$25/\text{bbl}} / (\text{PCPP}_{\text{WB}} / \text{PCPP}_{\text{petrochemical}})_{\text{US } \$50/\text{bbl}}$

*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).

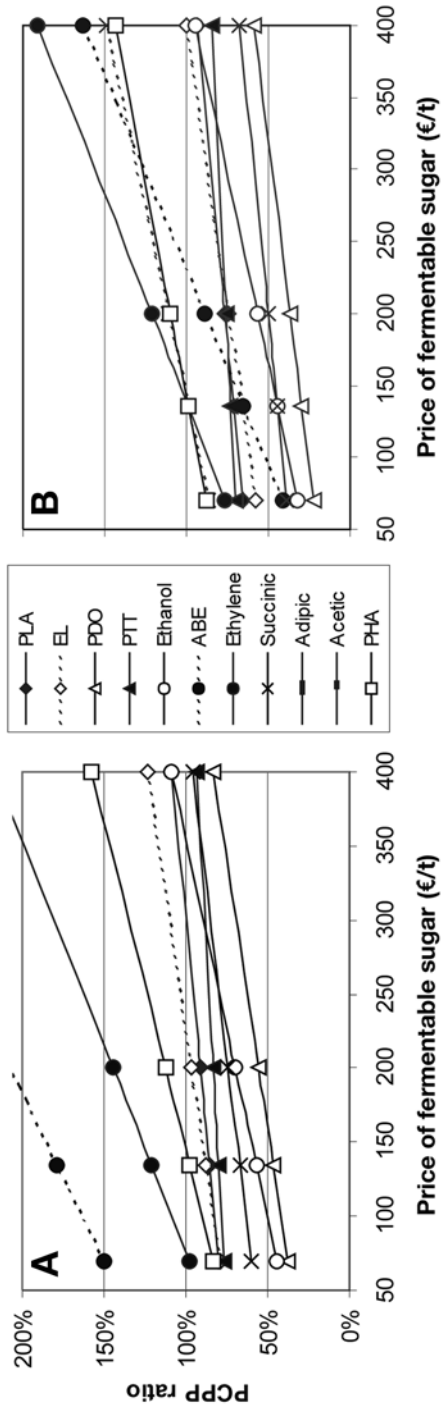


Fig. 7. Selected production cost plus profits (P CPP) ratios as a function of the sugar price for current (left) and future (right) technology at a high crude oil price (US\$50/bbl).

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 €/t and 16% (range: 10–30%) for a low sugar price of 70 €/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 €/t and by 25% (range: 10–35%) for the low sugar price of 70 €/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·h) instead of 50 g/(L·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 €/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 €/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 bio-based 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 bio-based 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 €/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 €/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.

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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.
5. Vink, E. T. H., Rábago, K. R., Glassner, D. A., and Gruber, P. R. (2003) *Polymer Degrad. Stab.* **80**, 403–419.
6. European Commission (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.
8. 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/>.