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Terms of Use

Impact of Biomass on Industry: Using Ethylene Derived from Bioethanol within the Polyester Value Chain

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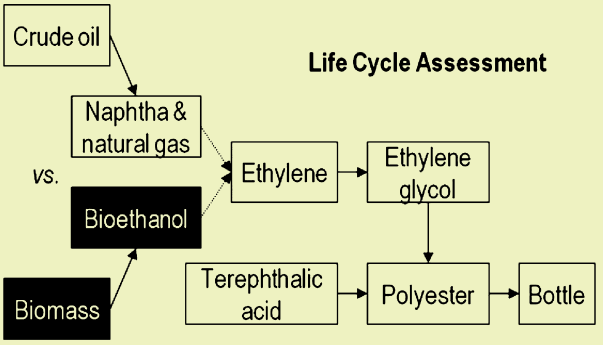
Supporting Information

ABSTRACT: Life cycle assessment has been used to investigate the environmental impacts associated with using ethylene produced from biomass, rather than from the processing of crude oil, in the production of polyethylene terephthalate (PET). The cases investigated were for polymer production and distribution facilities located either (i) in the United Kingdom (UK) or (ii) in the United States of America (USA). For these cases, the ethylene was assumed to be made in Brazil, starting from ethanol made from sugar cane, and subsequently converted to ethylene glycol before shipping. A further comparison was made for the UK-based plant in which ethylene glycol was produced from a hypothetical plant based in the UK using willow as the feedstock. Using the Brazilian ethylene glycol, the net reduction of greenhouse gas emissions, over a process using ethylene glycol from petroleum processing, was ∼28% when the final product was a 500 mL PET bottle. The accompanying reduction in total use of fossil fuel was ∼16%. Using ethylene glycol derived from willow biomass in the UK produced similar fossil fuel savings, however, a smaller 3.6% reduction in the greenhouse gases. Comparisons have also been made using other environmental impacts, e.g. acidification and eutrophication, for which the biomass systems are at a disadvantage. An economic assessment of the bioethanol to ethylene conversion process has demonstrated significant dependence on the feedstock cost and product price margin; the analysis suggests that such a process is unprofitable without incentives.



KEYWORDS: *Sustainability, Polyester, Bioethanol, Biomass, Life cycle assessment*

INTRODUCTION

Polyethylene terephthalate (PET) polyester is principally used to make textile fibers, bottles, and packaging films.[1] In terms of the annual tonnage produced, it is ranked third, behind polyethylene and polypropylene: 60 Mte was manufactured in 2011, an output which has grown between 5 and 7% per annum over the past decade.[2] Currently, PET is most commonly manufactured by the continuous polymerization of ethylene glycol and terephthalic acid.[3] Generally, both feedstocks can be derived from either naphtha or natural gas, with the proportion made from natural gas being larger in the United States of America (USA) than in the European Union (EU).[4] Of the annual tonnage of PET, ∼30% is used to make bottles, ∼67% is used in making fibres, and the remaining 3% for films and other uses.

Given that the environmental impacts of anthropogenic activities, such as global warming and resource scarcity, are a growing concern, there is increased pressure within the polyester industry to make production routes as sustainable as possible. One proposed route is to use biomass, rather than naphtha and natural gas, as the principal raw material for producing ethylene, and hence, ethylene glycol. Ethylene glycol accounts for 28 wt % of PET, based on raw material requirements. Thus this substitution has the potential to reduce the greenhouse gas emissions by replacing part of the fossil fuel requirement. An advantage of using biomass to produce ethylene glycol is that only minimal changes are needed to existing process plants because the reaction proceeds via an ethylene intermediate irrespective of starting raw material. While terephthalic acid routes from biomass are under development, they are not as close to commercialization as those for ethylene glycol. Thus, the focus in this paper is on ethylene glycol from biomass, despite the fact that terephthalic acid accounts for the larger proportion, i.e. 72%, of mass contributed to PET.

The objective of the research presented is to study the environmental impact, and economic feasibility, of using ethylene manufactured from bioethanol, rather than from naphtha and natural gas, in the production of PET. To do this, a life cycle assessment (LCA) has been undertaken to compare

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(i) the conventional process route (viz. with raw materials made from fossil fuel) and (ii) the modified process route (viz. using ethylene made from biomass). An important element in such an LCA is to define the system rigorously and, in particular, to define an appropriate functional unit, discussed later. It turns out that the life-cycle impacts of PET fibers are dominated by their use phase, e.g. the washing and drying of clothes.[5,6] Therefore, the present research concentrates on bottle-grade material where changes to the processing have a much greater influence on the product's overall environmental impact. The LCA did not include recycling or disposal, since the aim was to compare the impact of feedstocks on virgin PET.

While there have been previous studies of the LCA of PET from fossil fuel sources, one problem in comparing such research is the rather variable definition of the system under consideration and its boundaries. Also, there are no published comparisons with processes using biomass as a raw material. Roughly speaking, among existing studies on PET,[7,8] estimates of global warming potential are within the range 2.2−4.1 kg CO_2-eq/kg PET with a total fossil energy requirement of 69−95 MJ/kg PET. The ranges depend on the system boundaries drawn in the studies, e.g. the inclusion of the bottle molding process and the location of the production.

The route to obtain ethylene glycol from biomass involves producing ethanol, which is subsequently converted to ethylene. LCA studies exist for the production of ethanol from (i) first-generation, food crops, e.g. sugar cane,[9] sugar beet, corn, wheat, and potatoes; (ii) from second-generation lignocellulosic materials, e.g. willow[10] and switch grass; and (iii) from waste residues, e.g. corn stover, wheat straw, and molasses.[11−14] Most ethanol studies show savings on global warming potential and fossil fuel energy avoided. The main factors dominating the performance of bioethanol are crop productivity, climate, and the nature of the feedstock.[12] When assessing studies on bioethanol, the ranges for potential savings are large. This is owing to the different assumptions made regarding the cultivation, conversion, and allocation of byproducts.[14] Few studies, however, fully assess other environmental impacts; for those that do, bioethanol is typically at a disadvantage when compared to fossil fuels, with the key trade-offs being higher levels of acidification, eutrophication, and ozone depletion due to their use of nitrogen compounds in agricultural production.[12,14]

METHODS

The phases undertaken in the life-cycle assessment (LCA) were: (i) goal and scope definition, (ii) inventory analysis, (iii) impact assessment, and (iv) interpretation.[15,16] Here, the inventory analysis and impact assessment stages were aided by the process flowsheeting package Unisim and LCA software Gabi version 6, respectively.

Goal and Scope. The functional unit, a fixed reference quantity used as the basis for comparison between the different systems, was defined as one 500 mL PET bottle filled with a carbonated soft drink (CSD) after distribution to a supermarket. The mass of PET in the bottle was assumed to be 23.5 g.[17,18] The scenarios described later explore inter alia the effect of changes in geographical location of the final outlet for the bottles and the distances over which material is transported between the processes in the value chain. The boundary of the system studied encompasses all the processes directly involved with the production of the bottles (the foreground system) and also the secondary (background) processes. For background processes, e.g. the supply of electricity, existing databases were used, giving geographically dependent market averages of processes.

PET Value Chain. A value chain is defined here as the set of processes involved in producing the final functional unit from the defined starting materials, where each process can be considered to raise the value of the output over that of the input. The processes involved in the production of PET bottles from (i) conventional fossil-fuel sources and (ii) biomass are shown in Figure 1, with the difference between the routes being in the production of ethylene. Bioethanol displaces the naphtha or natural gas requirements for the production of ethylene. Irrespective of whether the ethylene is made from naphtha or bioethanol, it is oxidized to ethylene oxide using the oxygen-based direct oxidation process. The resulting ethylene oxide is reacted in excess water to yield ethylene glycol. Ethylene oxide and ethylene glycol manufacturing facilities are often contiguous, leading to energy

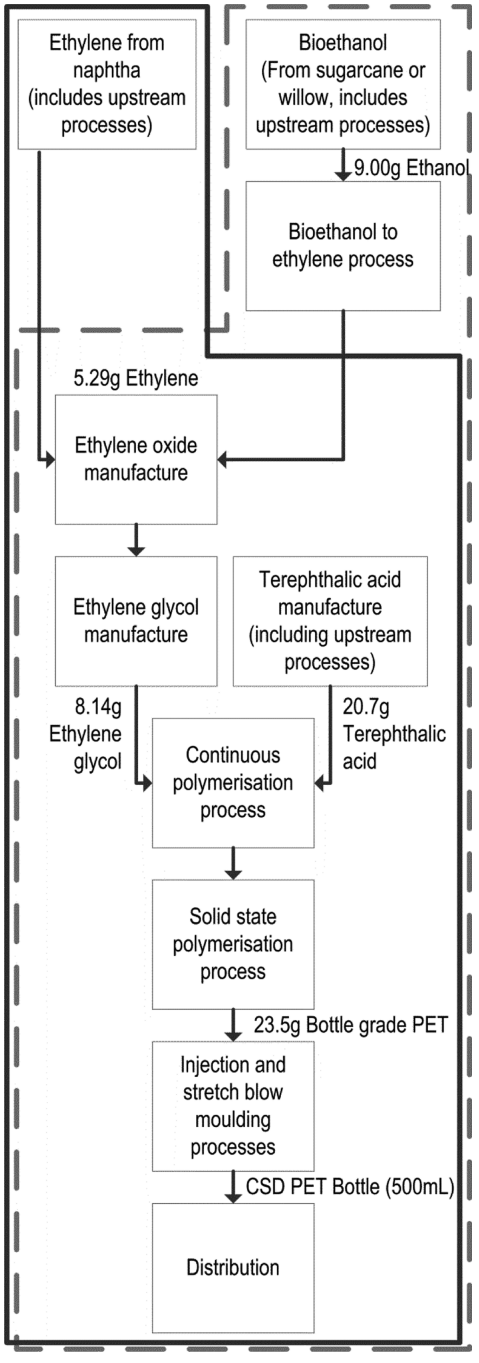


Figure 1. Polyester value chain including both conventional and biomass routes, which have been encompassed by their respective system boundaries for the life cycle assessment study.

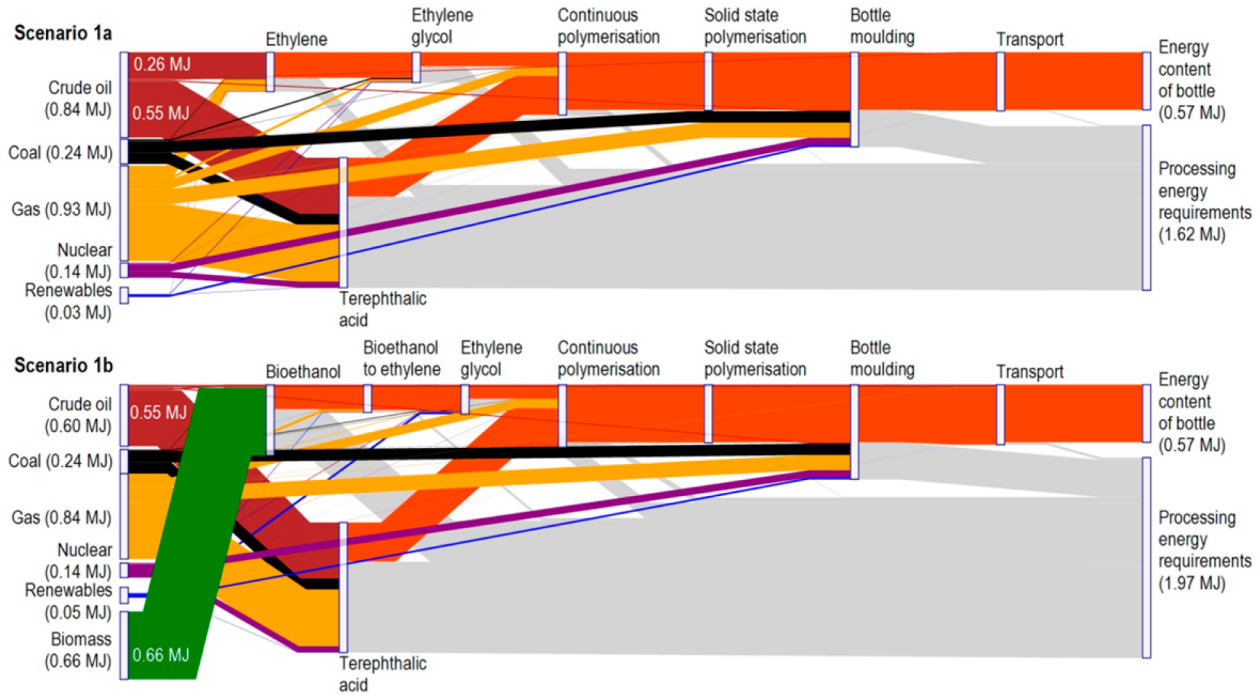


Figure 2. Sankey diagram showing the primary source of energy flows to each process for scenarios 1a and 1b.

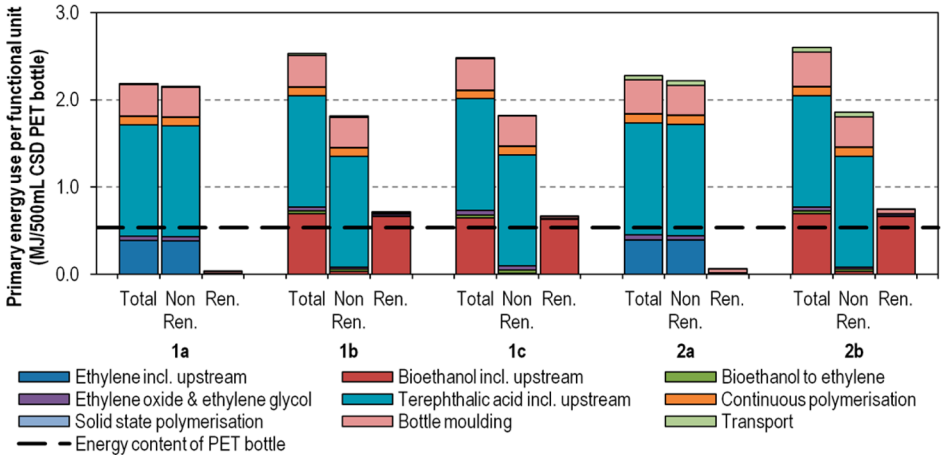


Figure 3. Energy use (MJ/functional unit) for each scenario; total energy requirements for the processes and distribution using renewable (Ren.) and nonrenewable (Non Ren.) sources.

savings by heat integration and avoiding the storage and transport of ethylene oxide, which is hazardous. In Figure 1, terephthalic acid is produced from the oxidation of *p*-xylene, which, in turn, is produced from the catalytic reforming of naphtha. As the focus of this study is on the impact of using biomass to produce, ultimately, the ethylene glycol, existing data concerning the environmental impacts of the production of terephthalic acid have been used. Purified terephthalic acid and ethylene glycol are combined in the continuous polymerization process. The molecular weight for bottle-grade PET is generally higher than that for fiber products and hence typically requires a further, solid-state polymerization stage, not needed for fibers.[19] The bottle-grade PET is injection molded into preforms and then stretch blow-molded to make bottles, which are filled and distributed.

For the inventory analysis, quantitative mass and energy balances were performed for the processes within the system. The detailed process flowsheeting, use of data sets, and methods of allocation are described in section 1 of the Supporting Information.

Location and Supply Chain. Two manufacturing locations for PET were considered, namely in the United Kingdom (UK) and the USA. For the UK, the terephthalic acid, continuous polymerization, and solid state polymerization were assumed to be collocated in northern England. In scenario 1a, ethylene glycol is conventionally sourced from The Netherlands and transported 600 km by ship to the UK polymerization sites. In the hypothetical scenarios, ethylene glycol is produced from sugar cane bioethanol in Sao Paulo, Brazil, and then transported 10 000 km by ship to the UK (scenario 1b) or ethylene glycol is locally produced in the UK from willow bioethanol (scenario 1c). It was assumed that PET would then be transported by truck an average distance of 300 km to bottle molding and filling facilities and a further 150 km to supermarkets via distribution centers.

For the USA, the continuous and solid state polymerization plants were assumed to be located in South Carolina. Terephthalic acid is transported 650 km by rail from Alabama to the polymerization facilities. Scenario 2a represents the conventional sourcing of ethylene glycol in Texas, which is then transported 1500 km to the PET facilities. In the hypothetical scenario 2b, ethylene glycol is produced from sugar cane bioethanol in Sao Paulo and the ethylene glycol is transported 9200 km by ship. It was assumed that PET pellets were

then transported on average 1000 km by truck to various bottle molding and filling facilities and a further 750 km by road to distribution centers for supermarkets.

In practice, owing to the diversity of supply chains, these scenarios (1a, 1b, 1c, 2a, and 2b) are only indicative of a supply chain for a PET CSD bottle. However, the scenarios have been chosen to capture most of the environmental impacts associated from the transportation of materials.

RESULTS AND DISCUSSION

Energy Distribution. To understand the overall flows of fossil and renewable fuels through the overall processes, Sankey diagrams were prepared and are shown in Figure 2 as energy flows for scenarios 1a and 1b (i.e., for PET plants located in the UK). As in all Sankey diagrams, energy is conserved and all the flows in a vertical section add to the same total quantity of energy entering at the left-hand side.[20] Figure 2 shows the primary sources of energy required for each of the processes as well as the energy content of the intermediates and the final product. The remaining energy from the balance is classified as the processing energy requirements. The results are shown for the functional unit, a 500 mL CSD PET bottle.

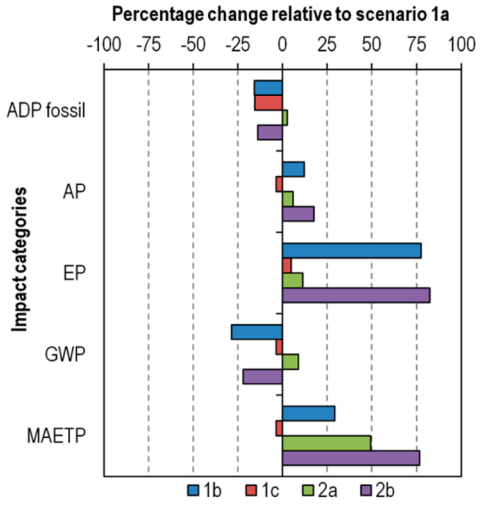
It can be seen that the substitution of the naphtha and natural gas feedstock results in a reduction of crude oil use and consequently an increase in biomass requirements, as expected. There is a 16% reduction of total fossil fuel requirement. For one 500 mL PET CSD bottle, Figure 2 shows that 0.26 MJ of crude oil can be avoided, but instead 0.66 MJ of biomass energy is required. It can also be seen that scenario 1b, in total, requires 16% more energy to produce the same bottle.

Figure 3 shows the total energy requirements in each scenario as well as energy requirements grouped by type, renewable and nonrenewable. Comparing the other bioethanol scenarios, 1c with 1a and 2b with 2a, there is a 16% reduction in fossil fuel use and a 16% increase in the total energy requirement. An important result from both Figures 2 and 3 is that the conversion of bioethanol to ethylene has, relative to the other processes, a small energy requirement, which does not affect, substantially, the overall energy balance. As a result, the global warming potential of the bioethanol to ethylene process is small, accounting for less than 3% of the total global warming potential for scenario 1b and, therefore, does not counteract the carbon dioxide savings of using biomass.

Impact Assessment. The impact assessment results are presented on the basis of the functional unit chosen, a 500 mL CSD PET bottle. The impact categories used are defined in Table S2 in the Supporting Information. Figure 4 shows the performance of scenarios 1b, 1c, 2a, and 2b relative to scenario 1a for the impact categories: fossil abiotic depletion potential, acidification potential, eutrophication potential, global warming potential, and marine aquatic ecotoxicity potential.

From Figure 4, using sugar cane bioethanol causes a reduction in the impact categories of global warming potential and fossil abiotic depletion potential compared with using ethylene from naphtha and natural gas. However, in every other impact category, there is an increase when sugar cane bioethanol is used. For the willow bioethanol, the difference for each impact category when compared to the conventional feedstock is less significant.

The impact categories represented in Table 1 were sensitive to small changes in the value chain. For example, the differences in electricity grid mix and transportation distances between the UK and USA for the conventional fossil fuel systems caused



Summary of values for base case, scenario 1a

Impact	Value	Units
ADP fossil	2.00	MJ
AP	3.22×10^{-4}	kg SO_2-eq
EP	2.25×10^{-5}	kg Phosphate-eq
GWP	0.092	kg CO_2-eq
MAETP	5.28	kg DCB-eq

Figure 4. Relative performance of scenarios 1b, 1c, 2a, and 2b with the reference scenario 1a in impact categories: fossil abiotic depletion potential (ADP fossil), acidification potential (AP), eutrophication potential (EP), global warming potential (GWP), and marine aquatic ecotoxicity potential (MAETP).

Table 1. Absolute Values for the Other Impact Categories Assessed for Each Scenario

scenario	ADP elements 10^{-9} kg Sb-eq	ODP 10^{-12} kg CFC R11-eq	POCP 10^{-5} kg ethene-eq	HTP 10^{-3} kg DCB-eq	FAETP 10^{-4} kg DCB-eq	TETP 10^{-4} kg DCB-eq
1a	7.51	2.69	5.38	9.51	2.66	32.4
1b	27.4	379	16.2	45.3	33.4	47.5
1c	54.2	41.0	5.05	9.41	2.51	33.2
2a	17.0	10.8	5.16	7.65	1.89	3.23
2b	31.3	386	16.1	43.5	32.7	18.5

large changes in impact categories. Comparing the scenarios, the bioethanol process often made the largest contribution to these impact categories.

Figure 5a–c shows for each scenario, respectively, the global warming potential, acidification potential, and eutrophication potential. Figure 5a shows the breakdown of global warming potential contributions by stage in the value chain shown in Figure 1. The total global warming potential for the production and distribution of a 500 mL CSD PET bottle using conventional fossil fuel, in the UK scenario 1a, is 0.092 kg CO_2-eq and, in the USA scenario 2a, 0.10 kg CO_2-eq. The use of bioethanol from Brazil resulted in a reduction of global warming potential of 28% for both the UK (1b) and the USA (2b). This reduction can be seen in Figure 5a to come from the carbon associated with bioethanol production which substitutes for the fossil fuel carbon used to produce ethylene glycol. Scenario 1c uses bioethanol from willow in the UK, and while this feedstock has a similar energy saving to sugar cane bioethanol, the global warming potential saving is much lower. This is because it was found in the study by Stephenson et al.[10] that there are larger emissions in some of the processing stages,

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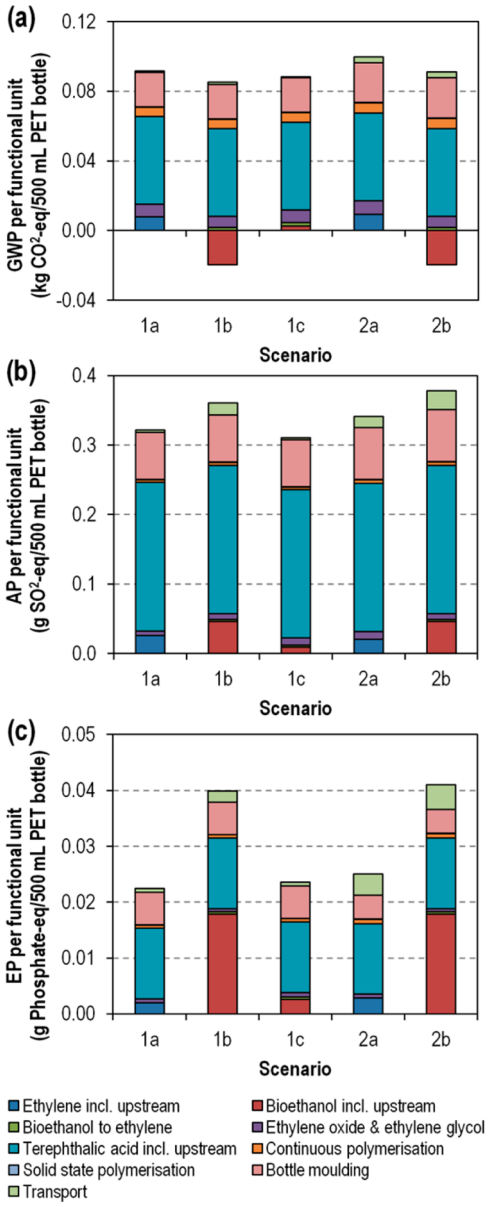

Figure 5. For each scenario, a detailed breakdown of the contribution from processes to (a) global warming potential (GWP), (b) acidification potential (AP), and (c) eutrophication potential (EP).

e.g. enzyme processing. Hence, comparing the willow bioethanol bottle in scenario 1c to the conventional scenario 1a, there is a 3.6% reduction in the global warming potential.

Interpretation. From the Sankey diagram in Figure 2, the substitution of the conventional feedstock results in a reduction of crude oil and natural gas use and consequently an increase in biomass requirement. Further, this route requires about 16% more energy in total to produce the same bottle, 2.53 MJ compared to 2.19 MJ for scenario 1a. So, while there is a beneficial reduction of fossil fuel energy use by using sugar cane biomass, there is also lower net energy efficiency in the conversion processes from biomass relative to the conversion from naphtha and natural gas. One limiting factor is the efficiency of the conversion from sugars to ethanol, e.g. maximum theoretical yield of 0.51 kg ethanol per kg glucose. Given that biomass is a renewable energy source, this does not impact the fossil fuel energy reduction, but it does mean that more biomass needs to be grown. This in turn results in larger impacts related to agronomy, as well as larger land areas devoted to sugar cane. Figures 2 and 3 also reflect the large energy requirements in terephthalic acid production and bottle molding, which are energy intensive processes. As a consequence, Figure 5a shows that these processes also make relatively large contributions to the global warming potential. Accordingly, because of the other processes involved, the global warming potential and fossil fuel energy savings of using biomass are lost to some extent when considering the end product, particularly in view of the fact that only 28% by mass of PET is ethylene glycol.

Figures 3 and 5a also demonstrate that the transporting of materials makes only a small impact in the global warming potential and energy requirement. This important result demonstrates that global scale supply chains for biomass are possible without significantly reducing the savings made. However, transport has other impacts, as discussed below.

A problem with using sugar cane ethanol is an increase in all of the impact categories, other than global warming potential. Two categories, acidification potential and eutrophication potential, are examined in more detail in Figure 5b and c. Figure 5b shows that the acidification potential has increased for the sugar cane bioethanol feedstock scenarios (1b and 2b) when compared to the conventional systems (scenarios 1a and 2a). The increase is attributable to both the bioethanol process and the transport of ethylene glycol over the long distance from Brazil. The contribution from the bioethanol processes arises in agronomy and particularly in the manufacture of the required fertilizers. Quirin et al.[14] also observed this impact for cultivated biomass. The willow bioethanol, scenario 1c, has a lower acidification potential; the study of Stephenson et al.[10] avoided considering synthetic fertilizers by using organic sludge from local water companies.

Figure 5c examined changes in eutrophication potential, arising largely as a result of the leaching of fertilizers into natural water courses. Figure 5c shows that growing sugar cane is particularly troublesome with respect to this impact. However, in contrast to sugar cane, the willow biomass does not need high applications of synthetic fertilizer and consequently its impact on eutrophication is much less. Transport is taken to affect eutrophication as a result of the release of nitrogen oxide emissions from engines and so the large transportation distances from Brazil to the UK or USA make a significant contribution to the eutrophication category for sugar cane ethanol. The process of conversion of bioethanol to ethylene, however, makes a negligible contribution to the acidification and eutrophication potentials.

Sensitivity. For the packaging of 500 mL of soft drink, the functional unit in this study, comparisons between the present results for energy and global warming potential and estimates for PET, aluminum, and glass made by Franklin Associates[8] are shown in Figure S6 in the Supporting Information. It should be noted that the study of Franklin Associates envisaged some recycled materials, so that PET bottles contained 23.5% recycled PET, aluminum cans 45.1% recycled aluminum, and glass bottles 30.7% recycled glass. However, it can be seen that PET bottles are competitive on a basis of global warming potential and fossil fuel energy use, a case strengthened when using the biomass derived ethylene as studied in scenario 1b.

The comparison among values for PET shows that the present estimates from scenario 1a for global warming potential of the PET bottle are within 6% of those estimated by Franklin

Associates, but there is a 30% difference with respect to energy use. On the other hand, if the functional unit for the present study were the polymer chip leaving the polymerization plant, a comparison can be made with a study by PlasticsEurope.[7] Here, there is a 29% difference in global warming potentials, but a smaller difference of 10% in energy use. Differences can arise due to the boundaries chosen, different allocation methods used, different process optimizations, or use of different supplementary data sets.

The sensitivity of using two different sources of bioethanol—from sugar cane and willow—source has been demonstrated with scenarios 1b and 1c in the results. However, as described earlier, there can be significant variation among bioethanol studies a on the boundaries chosen and the assumptions made. In order to assess how representative the reduction in greenhouse gases is from a particular biomass source, a sensitivity analysis has been conducted using the lower and upper ranges from Quirin et al.'s review for sugar cane bioethanol studies.[14] Table 2 shows a ±3% uncertainty in the global warming potential savings relative to scenario 1a.

Table 2. Sensitivity of the Sugarcane Bioethanol Study Used to Calculate the GWP Savings

	saving (kg CO_2-eq per kg ethanol)	GWP scenario 1b (kg CO_2-eq per 500 mL CSD bottle)	GWP cf. scenario 1a (%)
Ecoinvent	−2.19	0.065	−28
Lower[14]	−1.80	0.069	−25
Upper[14]	−2.87	0.059	−35

One study showed that deriving ethylene from corn bioethanol results in an increase in global warming potential when compared with ethylene from naphtha (+35%) or natural gas (+60%).[21] The key difference is the crop used, in this case, corn, which has fertilizer requirements approximately three times higher than sugar cane (corn 149 kg/ha, sugar cane 55 kg/ha).[22,23] Furthermore, sugar cane bioethanol has a much higher bioenergy output to fossil energy input yield ratio when compared to corn bioethanol, which means that corn is an energy intensive crop and it is therefore difficult to accomplish the desired reductions in carbon footprint.[12]

Two further sensitivities investigated concerning the difference between scenarios 1a and 1b are the conversion of bioethanol to ethylene and the effect of distance over which ethylene glycol is imported. These sensitivities were assessed with respect to the fossil energy required, global warming potential, acidification potential, and eutrophication potential as shown in Table 3.

Overall, the results are not very sensitive to the changes made, with respect to the base case, scenario 1b. However, lower conversion would result in more bioethanol being wasted, and it might be valuable to modify the process to include an ethanol recovery stage. As previously discussed, the results are not sensitive to the distance over which ethylene glycol is transported.

Wider Considerations. If PET packaging production worldwide were to use ethylene glycol derived from bioethanol instead of conventional processes, it would utilize 11% of the 1.0×10^8 m^3 annual bioethanol production capacity estimated for 2015.[24] World PET production in 2015 was projected using the average 6% annual growth rate from the 2011 60 Mte/y PET production while assuming the 30% fraction of PET for packaging use remained constant. Considering the land requirements for sugar cane bioethanol from Brazil, the 2011 PET production of 18 Mt/y is equivalent to approximately 17 000 km^2 of sugar cane cultivated land, at average harvests of 6.01 kg/m^2 and a conversion rate of 14.9 kg sugar cane per 1 kg bioethanol.[23,25] This land requirement amounts to 18% utilization of the 96 170 km^2 cultivated sugar cane land area in 2011 in Brazil.[26] This crude estimate serves to give some order of the amount of land required: of course, there are many conflicting requirements for such land, ranging from the need to produce ethanol for other industries wishing to switch from fossil-based feedstock to requirements for food production and the need to maintain the ecosystem, which are beyond the scope of the present study.

Water use is an important consideration for sustainability studies. In particular, when comparing the biomass feedstocks, the water use for sugar cane bioethanol is 15.5 kg, while that for willow bioethanol is 27.4 kg, on a per kilogram bioethanol basis.[10,23] The water use for cellulosic biomass is larger, primarily due to the pretreatment stages prior to fermentation. In both cases, no irrigation is required during cultivation, which is, in part, due to the geographical location (i.e., sufficient rainfall). When comparing scenarios 1b and 1c, with 1a, the total water usage was found to be similar, and the bioethanol processes contributed less than 10% to their respective scenarios. Other processes within the value chain had similar water requirements. For scenario 1b, the water use was assessed by excluding the Brazilian electricity grid mix given the significant quantity of hydroelectric power generation, for which the water use has been accounted for within the data set.

From an economic perspective, the investment needs to be profitable. Here, a basic economic assessment was performed, based on a reported capital investment of $278 million by Braskem to construct a plant to produce 200 kt/y ethylene from bioethanol.[27] A capital depreciation allowance, deductible before tax, of 15% on the total capital investment and a scrap value of 10% of the capital investment at the end of the 20 years plant lifetime were assumed. Corporation tax, without tax breaks, was estimated at 30% of profit, payable 1 year in arrears. On the basis of the process modeling and inventory analysis, 1.7 kg of bioethanol forms 1.0 kg of ethylene. With current bioethanol and ethylene prices at $674/t bioethanol and $1,246/t ethylene, respectively, the feedstock to product

Table 3. Sensitivity of LCA Results to Process Parameters

	details		change of impact category cf. base case (%)			
sensitivity	base case (scenario 1b)	change made (cf. base case)	fossil energy required	global warming potential	acidification potential	eutrophication potential
bioethanol to ethylene conversion	98.4%	93.4% (−5%)	+0.2	−1.4	+0.7	+2.3
ethylene glycol transport distance	10000 km	11000 km (+10%)	+0.1	+0.1	+0.4	+0.3

margin made on an ethylene basis would be \$99/t ethylene.[26,28] Other operating expenses were approximated based on the process modeling and typical costs of the utilities; however, the analysis shows that these operating expenses are insignificant compared to the feedstock costs.

Accordingly, the net present value shows a breakeven point after 20 years of production with a very low interest rate of 3%, giving no incentive from the industry to invest. The economics of this process indicate that while the facility does make a profit during the years of operation, the value added margin is not large enough to pay back the investment at a typical interest rate of 10%, only when the rate drops to 3%, is this possible. The most sensitive parameters in the analysis are the feedstock and product prices. A hypothetical case can be designed to determine the conditions required for such an investment to be profitable at a desired interest rate of 10% and also deliver an overall rate of return on the investment of 10%. Increasing the value added margin, by reducing bioethanol price and increasing ethylene price both by 22% results in the desired investment criteria being met. Under these conditions, a positive net present value and payback time is achieved after 4 years of production.

Such an assessment has illustrated that the economics are sensitive to feedstock and product price fluctuations owing to the small value added margins. Incentives such as tax cuts and grants would be necessary as the 22% feedstock and product price change is artificially high and unlikely to occur in the near future. These strategies are necessary unless the total investment cost can be reduced through further process integration and economies of scale.

Further Process Improvements. Currently, bioethanol production and the conversion of bioethanol to ethylene have been studied as independent processes. In the former, the ethanol is distilled to a purity of 95 wt %, but in the latter the ethanol would be diluted with water as discussed in section 1 of the Supporting Information. Integration of these processes could therefore reduce the distillation energy requirements if, for example, a 50 wt % ethanol stream were sent directly to the ethylene glycol process.

The functional unit defined was a 500 mL CSD bottle made of 23.5 g of PET. There is potential to reduce the mass to 18 g while maintaining the same strength performance.[17] Thus, using 23% less material results in a commensurate reduction of 23% in all impact categories. With no trade-offs, this technique delivers global warming potential reductions similar to those provided by substituting bioethanol from sugar cane. However, there is a limit to making lighter bottles without compromising the strength of the bottle. Combining the benefits of lighter bottles with bioethanol from Brazil, total savings in global warming potential and use of fossil fuel energy of, respectively, 45% and 35% are possible.

■ ASSOCIATED CONTENT

Supporting Information

Detailed modeling and flowsheeting undertaken for the inventory analysis, discussion of allocation methods and impact assessment categories, and a comparison with substitute drink containers. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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