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Economic performance and GHG emission intensity of sugarcane- and eucalyptus-derived biofuels and biobased chemicals in Brazil

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Abstract. Biomass feedstock can be used for the production of biofuels or biobased chemicals to reduce anthropogenic greenhouse gas (GHG) emissions. Earlier studies about the techno-economic performance of biofuel or biobased chemical production varied in biomass feedstock, conversion process, and other techno-economic assumptions. This made a fair comparison between different industrial processing pathways difficult. The aim of this study is to quantify uniformly the factory-gate production costs and the GHG emission intensity of biobased ethanol, ethylene, 1,3-propanediol (PDO), and succinic acid, and to compare them with each other and their respective fossil equivalent products. Brazilian sugarcane and eucalyptus are used as biomass feedstock in this study. A uniform approach is applied to determine the production costs and GHG emission intensity of biobased products, taking into account feedstock supply, biobased product yield, capital investment, energy, labor, maintenance, and processing inputs. Economic performance and net avoided GHG emissions of biobased chemicals depend on various uncertain factors, so this study pays particular attention to uncertainty by means of a Monte Carlo analysis. A sensitivity analysis is also performed. As there is uncertainty associated with the parameters used for biobased product yield, feedstock cost, fixed capital investment, industrial scale, and energy costs, the results are presented in ranges. The 60% confidence interval ranges of the biobased product production costs are 0.64–1.10 US\$ kg⁻¹ ethanol, 1.18–2.05 US\$ kg⁻¹ ethylene, 1.37–2.40 US\$ kg⁻¹ 1,3-PDO, and

1.91–2.57 US\$ kg⁻¹ succinic acid. The cost ranges of all biobased products partly or completely overlap with the ranges of the production costs of the fossil equivalent products. The results show that sugarcane-based 1,3-PDO and to a lesser extent succinic acid have the highest potential benefit. The ranges of GHG emission reduction are 1.29–2.16, 3.37–4.12, 2.54–5.91, and 0.47–5.22 CO_{2eq} kg⁻¹ biobased product for ethanol, ethylene, 1,3-PDO, and succinic acid respectively. Considering the potential GHG emission reduction and profit per hectare, the pathways using sugarcane score are generally better than eucalyptus feedstock due to the high yield of sugarcane in Brazil. Overall, it was not possible to choose a clear winner, (a) because the best performing biobased product strongly depends on the chosen metric, and (b) because of the large ranges found, especially for PDO and succinic acid, independent of the chosen metric. To quantify the performance better, more data are required regarding the biobased product yield, equipment costs, and energy consumption of biobased industrial pathways, but also about the production costs and GHG emission intensity of fossil-equivalent products. © 2019 The Authors. *Biofuels, Bioproducts, and Biorefining* published by Society of Chemical Industry and John Wiley & Sons, Ltd.

Supporting information may be found in the online version of this article.

Keywords: sugarcane; eucalyptus; biorefinery; biofuels; biobased chemicals; costs; GHG emissions; petrochemical reference

Introduction

To limit climate change and its impact on natural and human systems, *substantial and sustained* reductions in greenhouse gas (GHG) emissions are required.¹ The use of biomass for the production of bioenergy and biobased products is often highlighted as an effective way to reduce GHG emissions.^{2–5} Several integrated assessment studies^{6–9} have shown an increasing use of bioenergy and biobased products to reduce these emissions. The potential GHG emission reduction by biomass employment is influenced by the (biophysical) limits of biomass supply and the techno-economic performance of biobased supply chains.⁸ As indicated by Creutzig *et al.*,¹⁰ the global sustainable technical biomass supply potential is limited to 100–300 EJ year⁻¹. This value received medium agreement among scientists; biomass supply potential above 300 EJ year⁻¹ has low agreement among scientists. For comparison, the total global primary energy supply was ~570 EJ in 2015.⁵ For a successful biobased economy, the use of biomass should contribute to high GHG emission reductions, and it should be competitive with fossil alternatives. Efficient use of biomass is especially important given the restricted biomass supply. Greater insight into the production costs and GHG emission intensity of biobased products is therefore required.

The biomass potential for biofuel and biochemical production has been discussed extensively in the literature.^{2,11–14}

Some authors have performed a techno-economic analysis of biobased products considering a single product via different industrial pathways^{15–24} or multiple products via different industrial pathways.^{25–29} Others studies discussed the combined economic and GHG emission performance for a single product, for example ethanol.^{30–32} The main conclusions of these studies are that the major contributions to the total production costs of biofuels and biochemicals come from feedstock, energy consumption, capital investment, and operation and maintenance. However, it remains difficult to rank the economic and GHG emission performance of different biobased products; such studies are hardly comparable because they vary according to system boundaries, feedstock (type and composition), industrial scales, energy prices, and other relevant aspects and parameters (e.g. cost of maintenance, annuity, and labor). Furthermore, quantification of the GHG emissions intensity of biobased products is generally neglected, as in the studies mentioned above. In this respect, the literature is still limited on systematic combinations of a comprehensive techno-economic analysis with a GHG emissions intensity assessment to screen and select the most promising biobased products.^{33–38} Hence, the combination of these two factors (the lack of a harmonized assessment method for economics and GHG emissions, and the limited number of studies addressing these

aspects) makes it necessary to define both consistent methodological features (e.g. scope, context, functions, scale, assumption, etc.) and comparable process conditions prior to any evaluation of biobased products and processes.

In summary, the use of biomass for the production of biofuels and biobased chemicals faces two major challenges in the future. The first challenge is to have a high contribution to GHG emission reduction, especially given the limited land available for biomass cultivation. Secondly, the production costs of biobased production pathways should be able to compete with their respective fossil reference products, and with alternative biobased production pathways. To enable a fair comparison between different industrial processing pathways, a uniform approach should be applied to assess the economic performance and GHG emission intensity of different biobased products. The objective of this study is therefore to quantify and compare the production costs and GHG emission intensity of four relevant biobased chemicals using different biomass feedstocks, and compare these to their fossil reference product. The present study differs from prior studies as it quantifies both the production costs and GHG emission intensity of different biobased products using an uniform approach. The factory-gate production costs and GHG emission intensities are compared to their respective fossil references. Furthermore, the economic viability and GHG emission reduction potential are compared among the different biobased production pathways. To do this, the potential profit and GHG emission reduction are expressed per hectare of biomass feedstock production. The economic performance and net avoided GHG emissions of biobased chemicals depend on various uncertain factors, so this study considers uncertainty by means of a Monte Carlo simulation. A sensitivity analysis is also performed. These analyses are conducted to quantify the impact of the variation and uncertainty of the main economic and GHG emission parameters on the production costs and GHG emission intensity. The focus of this study is on the upstream and midstream part of the processing (cultivation, transport, and conversion), as further upgrading and distribution of biobased products is likely to be similar to the further upgrading and distribution of petrochemical platform products.³⁹ As the economic and GHG emission parameters are region specific, this study focus on one particular geographical region. Brazil has been selected as the case-study country because of its longstanding history in ethanol production, the expected expansion of biomass production, and the potential for the production of more advanced biobased supply chains.

Biomass feedstock description and biobased chemicals selection

Biomass feedstock selection

Brazil has a long history of first-generation ethanol production from sugarcane and it is currently the second largest bioethanol producer in the world.⁴⁰ The 2015/2016 harvest season yielded a total of 605 Mtonne of sugarcane⁴¹ for the production of sugar and ethanol on approximately 9 Mha.⁴² Furthermore, Brazil has strong potential to expand the sugarcane cultivation area, which is expected to increase by 6.4 Mha by 2021.⁴³ The high sugarcane yield, high industrial conversion efficiencies, and the co-production of electricity in the first-generation ethanol industry in Brazil have resulted in large GHG emission reductions – about 70% compared to gasoline according to the Joint Research Centre (JRC).^{44–46} The co-production of electricity is based on the utilization of bagasse (the left-over of sugarcane stalks after sugar extraction). Sugarcane bagasse can also be used in a second-generation process to increase the ethanol yield per tonne of sugarcane. However, this additional ethanol yield requires additional investment and reduces the electricity surplus.²⁰ In 2015, two industrial second-generation ethanol processing plants (designed for the production of 82 and 42 million liters ethanol per year) started operation in Brazil using sugarcane straw and bagasse.⁴⁷

The development and commercialization of second-generation industrial processing may also enable the use of eucalyptus as a feedstock for ethanol production. Currently, approximately 5.6 Mha of eucalyptus is planted,⁴⁸ mainly for the production of charcoal and pulp fiber, but also bioenergy.⁴⁹ The development of second-generation processing, especially the extraction and hydrolysis of sugars, can also be beneficial for the production of other sugar-derived products, such as succinic acid, polyethylene, or lactic acid.⁵⁰

Sugarcane and eucalyptus biomass will be considered as the two biomass feedstocks for industrial processing in this paper. Those biomass feedstocks are both largely cultivated in Brazil, and represent sugar and lignocellulosic biomass feedstock.

Biobased chemical selection

Sugarcane and eucalyptus can be used for the production of a wide variety of biofuels and biobased chemicals via biochemical or thermochemical industrial processing options. According to Gerssen-Gondelach,¹¹ the fermentation of sugars provides an attractive technology for the

production of biobased fuels and chemicals currently and in the longer term. The biobased products selected for more detailed analysis are therefore the output of a fermentation process (after sugar extraction). As a large range of potential biobased products can be produced via fermentation, multiple selection criteria have been applied to support the selection of relevant biobased production pathways. In this study, we use the following four selection criteria:

1. The biobased product should have a current or future market size of at least 100 ktonne per year to make a potentially substantial contribution to GHG emission reduction. As biomass use for energy and materials is considered to be an important GHG mitigation option, the production of the selected biobased chemicals should contribute to overall GHG emission reduction.
2. The biobased product should replace a fossil reference, either by direct or indirect substitution. To quantify the GHG emission reduction potential, the biobased product should have a petrochemical reference product with a known GHG emission intensity.
3. The biobased product should have received sufficient attention in the literature and sufficient data should be available to enable the analysis of the economic performance and GHG emission intensity.
4. The biobased product should be the main output of the industrial processing pathway to enable a direct comparison a fossil reference product. The common biobased production pathways should therefore be considered.

Table 1 provides an overview of biobased platform chemicals and their respective qualitative and quantitative scoring with regard to these criteria.

Based on the criteria and the scoring in Table 1, ethanol (C_2H_6O), ethylene (C_2H_4), 1,3-propanediol (PDO) ($C_3H_8O_2$), and succinic acid ($C_4H_6O_4$) were selected for an economic and GHG emission analysis. The four biobased products were assessed using first-generation (sugarcane) and second-generation (eucalyptus) processing. For ethanol, an integrated first- and second-generation industrial processing pathway was considered. Each production pathway consists of sugar extraction (and hydrolysis), fermentation of sugars to the final product, extraction, and purification. This purification step consists of a number of smaller processing steps. The configuration of the processing pathway of the first, second, and integrated first- and second-generation ethanol assumed in this study was based on Jonker *et al.*^{22,60} The specifications of the configurations of the ethylene processing pathways are described by Haro *et al.*²¹ The technical details of the processing

pathways of 1,3-PDO and succinic acid used in this study were derived from Anex and Ogletree (2006)⁷² and Efe *et al.*¹⁶ A simplified flowchart of the selected biobased platform chemicals and the main industrial processing steps is shown in Fig. 1. More information is provided about the different industrial processing pathways and the process characteristics of the selected biobased products in the supplementary information (SI.1).

Methods

This study aimed to quantify and compare the production costs and GHG emission intensity of ethanol, ethylene, 1,3-PDO, and succinic acid production using sugarcane and eucalyptus as biomass feedstock in Brazil, and compare them with their fossil references. To enable a comparison among the different biobased production pathways and their fossil references, a uniform approach and harmonized assumptions are applied. For this comparison, the production costs and GHG emission intensity are expressed in US\$ kg^{-1} final product and $kg CO_{2eq} kg^{-1}$ final product respectively. The GHG emissions reduction and potential total profit (both compared to their fossil-equivalent product) are expressed per hectare of feedstock production. These units enable comparison between the different industrial processing pathways and between the utilization of sugarcane or eucalyptus as biomass feedstock.

The focus of this analysis is on the industrial processing of sugarcane and eucalyptus to biobased products – e.g., from feedstock delivery to factory gate. To calculate the costs and GHG emissions of each pathway, an inventory of all mass and energy inputs and outputs of each of the industrial pathways is made (see the next section). This also includes the quantification of the biobased product yield (BPY) per tonne biomass input; either tonne sugarcane (TC) or dry tonne eucalyptus. The production costs of the biobased products are the sum of the costs for capital depreciation, biomass feedstock, energy, labor, maintenance, and other operational costs (see the section on ‘economic assessment’ below). The production costs of biobased products are compared with the prices of the fossil reference products. The GHG emissions of the biobased products include the GHG emissions of feedstock cultivation and transport, GHG emissions of other raw material consumption, operational GHG emissions, and GHG emissions related to energy demand or surplus. Greenhouse gas emissions related to direct and indirect land use change are not included. The GHG emissions of the biobased products are compared to those from the fossil-based equivalent products.

Table 1. Overview of potential biobased products with qualitative and quantitative scoring according to the selection criteria. In bold the biobased products selected for this study.

Chemical	Market potential	Fossil reference	Data availability	Biobased production route
Ethylene^a	127 Mtonne year⁻¹	Ethylene (naptha)	++	Fermentation, followed by dehydration of ethanol to ethylene
Ethanol^b	77 Mtonne year⁻¹	Gasoline (oil)	+++	Direct fermentation
Propylene ^c	53 Mtonne year ⁻¹	Propylene (byproduct of petrochemical processing)	–	Various options, including fermentation
Butadiene ^d	11 Mtonne	Petrochemical 1,3-butadiene	–	Via ethanol or via direct fermentation
Acetone ^e	3 Mtonne year ⁻¹	Acetone (coproduct of phenol production)	+/-	Co-product of ABE fermentation
Adipic acid ^f	2.6 Mtonne year ⁻¹	Petrochemical Adipic acid	--	Various pathways, for example the fermentation of glucose
Isopropanol ^g	2.3 Mtonne year ⁻¹	Via propylene	–	Fermentation
<i>n</i> -Butanol ^h	2.3 Mtonne year ⁻¹	<i>n</i> -butanol from mineral oil	+	Co-product ABE fermentation
Succinic acidⁱ	600 ktonne year⁻¹	Succinic acid / Maleic Anhydride	+/-	Fermentation
Lactic acid ^j	472 ktonne year ⁻¹	No direct; Lactic acid can produce different polymers.	+/-	Direct fermentation
1,3-PDO^k	125 ktonne year⁻¹	Petrochemical 1,3-PDO	+/-	Fermentation with genetically engineered organism
Isobutanol ^l	105 ktonne year ⁻¹	Isobutanol based on propylene	–	Yeast fermentation by genetically engineered organism
Itaconic acid ^m	41 ktonne year ⁻¹	Acrylic acid or maleic acid	–	Fermentation by means of fungi
3-HPA ⁿ	40 tonne	Unknown	–	Dehydration – fermentation (fermentation pathway not known)

^aEthylene has a global annual market volume of 127 Mtonne,⁵¹ of which currently a small fraction (0.2%) is biobased.¹³ Ethylene is not a direct fermentation product but can be produced via ethanol dehydration.⁵²

^bEthanol is an important biofuel replacing gasoline. In 2015 global annual ethanol production increased $\pm 4\%$ to 98.3 billion liters; at the same time production in Brazil reached a record of 30 billion liters.⁴⁷ Around 18% of the ethanol production is for non-energy applications.⁵⁰ For ethanol production various publications assess the economic performance of first, or second generation industrial processing. (e.g.^{53–55}).

^cPropylene is an important platform chemical with an annual market volume of 53 Mtonne.³⁹ The production from biobased feedstock can occur via different processes (via ethylene, *n*-butanol, acetone, isopropanol, or via propane).¹²

^dButadiene can be produced either via ethanol or via direct fermentation.¹²

^eWith a current production capacity of 3 million tonne year⁻¹,⁵¹ the demand for new production capacity is limited as acetone is a co-product of phenol, which is economically more attractive.^{51,56}

^fNo detailed economic data was found for the production of adipic acid. The annual market of 2.6 Mtonne is based on Straathof *et al.*⁵¹ There are various production pathways, including fermentation of glucose.⁵¹

^gIsopropanol is mainly used as solvent with a total production around 2.3 Mtonne,⁵¹ and it is produced using propylene as feedstock.⁵¹ Isopropanol via sugar fermentation is currently under development.¹²

^h*n*-Butanol is a co-product of ABE fermentation¹³, with an annual market of 2.3 Mtonne.¹²

ⁱThe estimated global market is projected to reach 599 ktonne in 2020.⁵¹ The market for succinic acid (fermentation product)¹² and its derivatives can even reach 6.2 Mtonne year⁻¹ (theoretical upper limit) if succinic acid replaces all other specific end-use applications.⁵⁷ Important to note is that the study by Harmsen *et al.*⁵⁸ estimated the succinic acid production at only 40 kton year⁻¹, of which 1 kton year⁻¹ was biobased, in 2013. However, the study by Weastra estimated the potential increase in production capacity of biobased succinic acid to be 637 kton year⁻¹ in 2020.⁵⁷

^jLactic acid is currently mainly used for the production of polylactic acid (PLA).⁵¹ The entire lactic acid production of 472 ktonne is biobased.¹³

^kRecently, 1,3-PDO production by fermentation of glucose and glycerol has been developed.^{51,56} Studies estimated that a large fraction of the current production (125 ktonne¹²) is biobased.^{12,13} Novel production pathways include the fermentation with use of genetically engineered yeast.⁵⁶

^lThe current market for isobutanol (105 ktonne¹³) is approximately 21% biobased.¹³ Novel production pathways include the fermentation with use of genetically engineered yeast.¹³

^mItaconic acid is assumed to be 100% biobased production,¹³ with the use of fungi during fermentation,⁵⁹ and a current market volume of 41 ktonne.¹² With the wide diversity of substitution possibilities the total market volume is estimated as 6.2 Mtonne.⁵⁷

ⁿ3-Hydroxypropionic acid (HPA) is a C₃ platform chemical with derivatives for the commodity as well as the specialty chemicals market.⁵⁶ At the moment production is limited to 40 tonne.¹³ The specific fermentation pathways are not known.⁵⁶

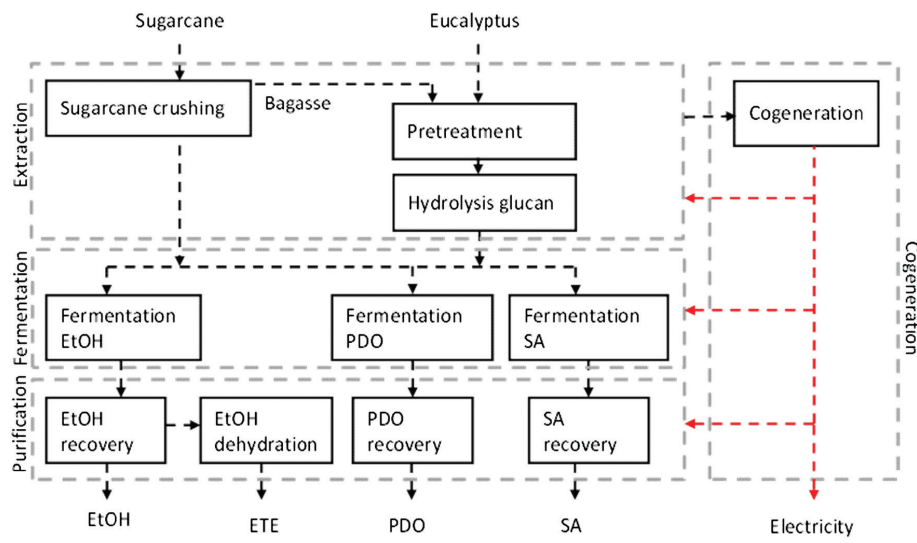


Figure 1. Simplified flowchart of the selected biobased platform chemicals and the main industrial processing steps, including the cogeneration unit for process steam and electricity.

To enable a uniform comparison, the costs and GHG emission intensity of biomass feedstock supply, the scale of the industrial processing plant, the costs and GHG emission intensity of energy use, and the main economic assumptions are equal for the different biobased processing pathways. Due to the considerable uncertainty of the costs and the GHG emissions of the (novel) biobased pathways and their fossil references, both a sensitivity analysis and an uncertainty analysis are performed. The results of these analyses quantify the potential range of production costs and GHG emissions of the biobased products given the uncertainty in the key parameters. The different ranges are compared to the ranges in factory-gate production prices and GHG emission intensities of the fossil reference products, which are based on a literature review.

Combining the production costs, fossil reference price, BPY, and the average biomass yield per hectare in Brazil results in the potential net profit per hectare per year. Similarly, the net GHG emission reduction of each biobased processing pathway is calculated per hectare.

Mass and energy inventory

The mass and energy inventory includes the calculation of the BPY, and the inventory of mass inputs and heat, steam, and electricity consumption or electricity surplus. The BPY per tonne of biomass feedstock is determined using the feedstock composition, maximum stoichiometric conversion, and the industrial processing efficiencies – see Eqn (1). First, the amount of available sugars in the sugar-

cane and eucalyptus is quantified, based on published data regarding biomass composition. The stoichiometric mass efficiency is based on the simplified chemical equation of the conversion process, and represents the maximum efficiency (theoretical upper limit) of conversion of sugars to the selected biobased chemical. A number of factors limit the amount of BPY that can be produced per tonne of biomass feedstock, namely efficiency of sugar extraction or biomass pretreatment, fermentation, and purification of the final product. The aggregated efficiencies of these main processing steps represent the mass conversion or processing efficiency of the individual steps and are based on available literature regarding conversion and product yield.

$$BPY = S \cdot \eta_{Ex} \cdot \eta_{Fer} \cdot \eta_{max} \cdot \eta_{RP} \tag{1}$$

Item	Description	Unit
BPY	Biobased product yield	kg biobased product/tonne biomass feedstock
S	Sucrose or glucose content per tonne biomass feedstock	kg sugar/tonne biomass feedstock
η_{Ex}	Sugar extraction efficiency	%
η_{Fer}	Fermentation efficiency	%
η_{max}	Maximum conversion efficiency	%
η_{RP}	Recovery and purification efficiency	%

An inventory of the major mass and energy inputs is made, which specifies the demand for yeast, chemicals, steam, fuel, and electricity for the extraction, fermentation and recovery of the selected biobased chemicals. This inventory is based on the available literature regarding mass and energy inputs and is normalized to tonne biomass feedstock input or kg final biobased product. Minor inputs such as lubricants are not quantified but are included in the operational costs via a fixed percentage of the fixed capital investment (FCI) as annual costs for minor industrial inputs.

Economic assessment

A discounted cash-flow spreadsheet is employed to calculate the production costs of biobased products (BPC) of the different industrial processing pathways producing ethanol, ethylene, 1,3-PDO and succinic acid. The cash flows include the expenses for sugarcane or eucalyptus feedstock, investment, maintenance, operational expenses, labor, and energy inputs – see Eqn (2). The FCI of an industrial processing pathway is the sum of the costs for the different processes required to produce the specific biobased product. For each processing step, as distinguished in Fig. 1, the equipment costs (EC) are taken from literature, scaled with the scaling factors (see Eqn (3)), and multiplied by the appropriate Lang factor (LF) (ratio of FCI to the total purchased equipment costs). The annual expenses for minor operational inputs, maintenance, and labor are calculated as a fixed annual percentage of the FCI. The annual production of the biobased product of an industrial plant is the product of BPY, the scale of the industrial processing plant, and annual operational hours (see Table 5) and (SI.2). The process energy demand is partly met by the co-generation unit. It is assumed that energy consumption that is not covered by the cogeneration unit is purchased externally. The energy costs are based on the prices for externally purchased steam, fuel, and electricity. All costs are calculated in 2016 US dollars.

$$BPC = \frac{(\alpha \cdot FCI) + OI + M + L}{BPY \cdot cap \cdot hours} + \frac{F}{BPY} - \left((E_{production} - E_{consumption}) \cdot E_{price} \right) \quad (2)$$

Abbreviation	Description	Unit
BPC	Production costs of biobased product	US\$ kg ⁻¹ biobased product
α	Capital recovery factor	%
FCI	Fixed capital investment	US\$

OI	Annual operational inputs	US\$ year ⁻¹
M	Annual maintenance costs	US\$ year ⁻¹
L	Labor expenses per year	US\$ year ⁻¹
CPR	Co-product revenues per year	US\$ year ⁻¹
BPY	Biobased product yield	kg biobased product per tonne sugarcane or kg biobased product dry tonne eucalyptus
Cap	Industrial capacity	TC h ⁻¹ or dry tonne h ⁻¹
Hours	Annual operational hours of the industrial plant	Hours year ⁻¹
F	Feedstock costs	US\$ per tonne sugarcane or US\$ or dry tonne eucalyptus
E _{production}	Energy production in cogeneration unit	kWh kg ⁻¹ biobased product
E _{consumption}	Energy consumption of different processing steps	kWh kg ⁻¹ biobased product
E _{PRICE}	Energy price	US\$ kWh ⁻¹

$$FCI = \sum \left(\text{Base EC} \cdot \left(\frac{\text{Scale}}{\text{Basescale}} \right)^{SF} \right) \cdot LF \quad (3)$$

Abbreviation	Description	Unit
FCI	Fixed capital investment	US\$
LF	Lang factor	[—]
EC	Equipment costs of the equipment installed	US\$
Base EC	Equipment costs of the base scale	US\$
Scale	Scale of equipment	Various units; e.g. tonne h ⁻¹
Base scale	Base scale corresponding to the base EC	Various units; e.g. tonne h ⁻¹
SF	Scaling factor of installed equipment (until it reaches maximum scale)	[—]

GHG emission intensity

Greenhouse gas emission calculation methodologies for different types of bioenergy have been developed for decades.^{61–64} Some methods are included in legislation in, for example, the EU and the US,^{61–63} and have very detailed and clearly defined rules on, for instance, how to deal with allocation, and what the fossil reference is for comparison. For the life-cycle assessment of the production of biobased and fossil chemicals, ISO standard 14044 has been developed.⁶⁴ This is used as basis for the GHG emission quantification in this study.

This study focuses on biobased processing pathways with one main output: ethanol, ethylene, 1,3-PDO, or succinic acid. Other outputs of the production pathways are considered as byproducts. When considering one main product, the displacement method is usually selected as the allocation method in life-cycle analysis.⁴⁴ This means that for byproducts of industrial processing pathways, the potential displacement of GHG emissions are credited to the main output of the biobased production pathways. An electricity surplus results in GHG emissions being avoided due to the substitution of Brazilian electricity from the grid. Avoided GHG emissions are credited to the main biobased product output.

Greenhouse gas emissions from biomass supply are included through the use of data published in other studies for sugarcane and eucalyptus cultivation and transport, combined with the biobased product yield. Industrial GHG emissions include the inputs for industrial processing and their respective GHG emission intensity. By summing the feedstock supply, industrial processing, and energy GHG emissions and normalizing the results to the functional unit (i.e. 1 kg ethanol, ethylene, 1,3-PDO or succinic acid), the GHG emission intensity of biobased products is calculated – Eqn (4).

$$\text{GHG} = \frac{F_{\text{GHG}}}{\text{BPY}} + IP_{\text{GHG}} - \left((E_{\text{production}} - E_{\text{consumption}}) \cdot E_{\text{GHG}} \right) \quad (4)$$

Abbreviation	Description	Unit
GHG	Greenhouse gas emission intensity of biobased product	kg CO _{2-eq} kg ⁻¹ biobased product
F _{GHG}	Feedstock GHG emission intensity	kg CO _{2-eq} tonne ⁻¹ biomass
IP _{GHG}	Industrial processing GHG emissions	kg CO _{2-eq} kg ⁻¹ biobased product
E _{production}	Energy production in cogeneration unit	kWh kg ⁻¹ biobased product

E _{consumption}	Energy consumption of different processing steps	kWh kg ⁻¹ biobased product
E _{GHG}	Greenhouse gas emissions of energy consumption	Kg CO _{2-eq} kWh ⁻¹
BPY	Biobased product yield	kg biobased product per tonne biomass

Fossil reference

The production costs and GHG emission intensity of biobased ethanol, ethylene, 1,3-PDO and succinic acid are compared to the costs and GHG emissions of the equivalent petrochemical reference products. As shown in Table 1, petrochemical gasoline, ethylene, 1,3-PDO, succinic acid and maleic anhydride are selected as fossil reference products. Ethanol is considered as direct substitution for gasoline, as 82% of the ethanol production is for energy applications.⁵⁰ Ethanol is therefore compared to gasoline based on the energy content. Biobased ethylene is assumed to replace petrochemical ethylene. Similarly, biobased 1,3-PDO and succinic acid are assumed to replace their fossil-based counterparts. However, as the fossil reference platform chemical for succinic acid depends on its derivate products, both petrochemical succinic acid and maleic anhydride are selected. The production costs and GHG emission intensity of the biobased products are compared to their equivalent fossil reference product on a factory-gate basis.

Production costs of petrochemical products are not publicly available. As a proxy for factory-gate petrochemical cost ranges, a direct relationship between crude oil prices and the price of petrochemical derivatives is therefore considered in this study. To determine the price range of a petrochemical reference product, the price is first determined based on available literature and databases. This base value is then multiplied by the range in oil prices of the last 10 years and the price growth factors for basic chemicals or petroleum products. The price growth factors indicate the variation in price of a commodity with a doubling of the price of crude oil⁶⁵. The basis for using growth factors is that the prices of petrochemical commodities increase with increasing oil prices, as supported by the relationship of ethylene prices in relation to crude oil prices.²¹

The range in GHG emission intensity of petrochemical products is based on values found in the literature. It is important to note that the GHG emission intensity, expressed as CO_{2eq} per kg product, includes the factory-

gate GHG emissions and the combustion GHG emissions at the end-of-life use of the products. The GHG emissions related to combustion are based on the embedded fossil carbon in petrochemical products. The lowest and highest value for the GHG emission intensity of the fossil reference products found in literature are plotted in the results. This depicts the potential range of the GHG emission intensity of fossil reference products. It includes the variation in GHG emission intensity values due to different geographical regions and different Life Cycle Analysis (LCA) allocation methods. The GHG emission reduction potential of a biobased production pathway is the difference between the GHG emission intensity of the fossil product and the biobased product.

Sensitivity and uncertainty analysis

In this study, data are taken from other publications to determine the BPY, production costs, and the GHG emission intensity of the biobased products. The data are prone to uncertainty, and vary according to their geographical and temporal scope. The uncertainty of one or multiple parameters cannot be directly translated to the potential variation in production costs or GHG emission intensity. The impact of the variability and uncertainty of the different input parameters on the final result is addressed by a sensitivity analysis and an uncertainty analysis.

First, the sensitivity of the production costs and GHG emission intensity to variations in the most prominent parameters is determined by a single-parameter sensitivity analysis. The parameter variations are based on the ranges of the different key parameters found in the literature. An early screening showed that the key parameters in this study affecting the production costs were the feedstock costs, biobased product yield, total investment, industrial scale, and the price of the energy consumed. For the GHG emission intensity, the BPY and the GHG emissions of feedstock supply and process energy are considered key variables. The results of the sensitivity analysis show the impact of variation in a single parameter on the production costs and GHG emission intensity of each biobased product.

Second, a Monte Carlo simulation is performed to quantify the confidence intervals of the production costs and GHG emission intensity of biobased products. Each variable has a specific probability distribution which is used in the Monte Carlo analysis. The distribution for each parameter is based on the available data, and is discussed in the following section. In the Monte Carlo simulation, all key input parameters are simultaneously varied in

accordance with their probability distribution. The results of the Monte Carlo simulation are probability distributions for the production costs and GHG emission intensity of the biobased products. These results are plotted for a 60%, 80%, and 90% probability range, and compared to the ranges of the prices and GHG emission intensities of their fossil reference product. This selection of 60%, 80%, and 90% was made to illustrate the degree of (un)certainty of the results.

Data input

This section is structured according to the data requirements for determining the BPY, energy use, economic data, GHG emission data, and fossil reference. Each subsection describes the data used in the analysis, the uncertainty associated with these data, and the data sources. For the key parameters considered in the Monte Carlo analysis, uncertainty or variation is described as having a normal, triangular, or uniform distribution. A normal distribution is a common probability distribution. A uniform distribution is one in which all intervals have the same probability. A triangular probability distribution is one in which the triangle is shaped by the upper and lower limit, and a mode.

Industrial conversion efficiency to biobased products

Table 2 includes the mass efficiencies of fermentation, maximum stoichiometric mass yield, and the product recovery and purification efficiency, to determine the BPY for ethanol, ethylene, 1,3-PDO, and succinic acid. The distribution for the BPY is determined based on the ranges of the different process efficiencies, and their probability distribution.

Sugarcane ethanol production is an established industry with multiple companies and a large number of industrial processing facilities installed.^{50,60} After decades of operational experience with sugarcane-to-ethanol industrial facilities, several studies have discussed the historic development of industrial efficiency,^{66,78} surveyed operational industrial plants annually,^{79–81} and studied current economic and GHG emission performance.^{20,44,45,82} The BPY,^{66,83} and steam and electricity consumption²⁰ can therefore be calculated with a high level of certainty.

The eucalyptus-to-ethanol production process is proposed in different studies.^{22,55,84} However, as far as we are aware, no industrial plants have been constructed using eucalyptus as feedstock. Although the scientific body is

Table 2. Extraction, fermentation, and product recovery efficiencies and resulting BPY (in bold) for the different industrial processing pathways.

Parameter	Unit	Base value	Range	Probability distribution	Reference
Sucrose content SC	Kg TC ⁻¹	145 ^a	130–165 ^b	Uniform	20
Sucrose extraction	%	96	95–97 ^c	Uniform	66
Fermentation to ethanol	%	92	88–94.5 ^d	Uniform	22
Stoichiometric ethanol	%	51 ^e	—	—	67
Distillation	%	99	97–99.5 ^f	Uniform	66
BPY 1G ethanol	Kg TC⁻¹	64	49.5–75.7 (100%) 56.0–73.0 (90%)	Normal (mean 63.4, Std Dev 4.65)	
Pretreatment of lignocellulosic biomass	%	95	90–100 ^g	Uniform	68
Hydrolysis of lignocellulosic biomass	%	80	75–90 ^h	Uniform	68
BPY 1+2G ethanol	Kg TC⁻¹	91	71.6–101.5 (100%) 78.1–94.6 (90%)	Normal (mean 86.2, Std Dev 5.07)	
Glucan content EU	Kg dry tonne ⁻¹	495	495	—	55
BPY 2G ethanol	Kg dry tonne⁻¹	243	192.4–281.1 (100%) 203.8–267.1 (90%)	Normal (mean 234.8 Std Dev 19.74)	
Stoichiometric ethylene	%	61	—	—	55
Ethanol dehydration	%	98	96–100% ⁱ	Uniform	21
BPY 1G ethylene	Kg TC⁻¹	37	31.1–37.9 (100%) 33.5–42.5 (90%)	Normal (mean 38.5, Std Dev 2.84)	
BPY 2G ethylene	Kg dry tonne⁻¹	140	114.2–170.0 (100%) 121.6–160.0 (90%)	Normal (mean 140.3, std dev. 12.0)	
Stoichiometric 1,3-PDO	%	84	—	—	
Fermentation 1,3-PDO	%	61	55–67 ^j	Uniform	
Recovery 1,3-PDO	%	90	80–100 ^k	Uniform	19
BPY 1G 1,3 PDO	Kg TC⁻¹	62	45.4–88.1 (100%) 53.0–76.7 (90%)	Normal (mean 65.0, std dev. 7.2)	
BPY 2G 1,3-PDO	Kg dry tonne⁻¹	207	140.0–272.4 (100%) 162.0–241.5 (90%)	Normal (mean 198.6, std dev. 24.1)	
Stoichiometric succinic acid	%	112	—	—	
Fermentation succinic acid	%	75	62–110 ^l	Uniform	
Recovery succinic acid	%	92	70–95 ^m	Uniform	
BPY 1G succinic acid	Kg TC⁻¹	107	54.0–159.2 (100%) 70.1–133.3 (90%)	Normal (mean 99.5, std dev. 19.4)	
BPY 2G succinic acid	Kg dry tonne⁻¹	326	169.1–497.5 (100%) 216.1–416.5 (90%)	Normal (mean 303.0, std dev. 61.0)	

^aBase value sugar content of sugarcane similar to the study by Dias.²⁰

^bSugar content varies within a harvest season, between genotypes, and between years.^{69,70}

^cIn recent decades the extraction yield increased from 92% to 96%, with 97.5% as the upper limit.⁶⁶

^dThe fermentation yields increased from 88% to 91%, with 93% being the upper best practice.⁶⁶ Due to the production of byproducts, 94.5% is considered the upper practical limit.⁶⁷

^eThe maximum stoichiometric mass conversion efficiency of sugar to ethanol is 51%.⁶⁷

^fDue to higher ethanol content in fermentation broth and technology improvement, the distillation of ethanol has now reached 99% efficiency.⁶⁶

^gDuring pretreatment small amounts of sugars are converted to other products.⁶⁸

^hHydrolysis includes the reaction of glucan to glucose (ratio 1–1,11). A small fraction of the glucan is converted to glucose oligomer and cellobiose.⁶⁸

ⁱThe dehydration of ethylene is reported to have a high mass conversion efficiency.^{17,21} Due to the lack of data about the maximum practical limit, the upper limit is set to 100%.

^jThree studies^{71–73} use 0.51 kg kg⁻¹. No information was found on the range. A variation of 10% was assumed due to the agreement between earlier mentioned studies. See also potential increase in fermentation yield as used in the study of Stegmann.⁷⁴

^kData is lacking; a range of 80–100% is assumed to assess the potential impact of the variation in the efficiency of recovering on the final results. Include various steps; different filtration steps, ion-exchange, evaporation, distillation, and hydrogenation.^{19,75}

^lSee the review by Cheng *et al.* (2012)⁷⁶ which reported yield (g g⁻¹ of succinate on glucose).

^mDifferent extraction rates have been published and commonly vary between 70 and 95%.⁷⁷ The latter is a chain of extraction processes.

extensive, the range found for ethanol yield of lignocellulosic feedstock is considerable, with medium uncertainty regarding the BPY.⁵³

The production pathway of ethylene via ethanol (ethanol dehydration to ethylene) is currently being commercialized by several companies.⁵⁰ No information was found on the operational yields, costs, or GHG emissions of these industrial plants. Desktop studies for ethanol dehydration to ethylene all show high BPY (all over 97% of stoichiometric efficiency).^{52,85,86} The ethanol to ethylene production process is therefore qualified as having a low uncertainty level, but the uncertainty level of the entire production pathways depends on the uncertainty of ethanol production as well.

The detailed published data found for the production of succinic acid from sucrose is limited to the study by Efe *et al.*¹⁶ The efficiency of the industrial processing steps is

based on Efe *et al.*¹⁶ No techno-economic data were found in the literature for the production of 1,3-PDO using sugarcane or eucalyptus as feedstock. Conversion rates of sugar to 1,3-PDO in lab experiments are used to calculate the BPY of 1,3-PDO production. Uncertainty is therefore considered high for the BPY of 1,3-PDO and succinic acid production.

Energy consumption of various configuration

Table 3 lists the energy demands or energy surpluses of the different industrial processing facilities. Several studies have been published that provide data regarding electricity production, use, and surplus.^{20,80} These studies show little variation in surplus electricity. For ethylene production, the studies of Haro *et al.*²¹ and Nitzsche *et al.*¹⁷ are con-

Table 3. Energy demand and surplus energy for the processing of sugarcane into ethanol, ethylene, 1,3-PDO and succinic acid.

Process	Value	Unit	Reference
Boiler efficiency	90	%	20
Steam production sugarcane bagasse	616 ^A	kg steam TC ⁻¹	Own calculation
Steam production eucalyptus	2579 ^B	kg steam dry tonne ⁻¹	Own calculation
Steam to electricity conversion	3 ^Z	kg steam kWh ⁻¹	89
Steam use cane reception	171 ^B	kg steam TC ⁻¹	90
Electricity own use cane reception	16 ^C	kWh TC ⁻¹	20
Steam use ethanol distillery	107 ^B	kg steam TC ⁻¹	90
Electricity use ethanol distillery	30 ^C	kWh TC ⁻¹	20
Electricity ethanol dehydration	0.21 ^D	kWh L ⁻¹ ethanol	17,21
Fuel ethanol dehydration	1.34 ^E	MJ L ⁻¹ ethanol	21,92
Steam demand for ethanol dehydration	3.96	MJ kg ⁻¹ ethylene	91
Electricity consumption for 1,3-PDO fermentation and purification	0.0323 ^J	kWh kg ⁻¹ PDO	87
Natural gas use for 1,3-PDO fermentation and purification	15.13 ^K	MJ kg ⁻¹ PDO	87
Succinic acid natural gas use	3.46	MJ kg ⁻¹ succinic acid	88
Succinic acid steam use	20.15	Kg MP steam kg ⁻¹ succinic acid	88
Succinic acid electricity use	0.538 ^I	kWh kg ⁻¹ succinic acid	88

^AUsing a fiber content of 14% (140 kg dry bagasse TC⁻¹), moisture content of 50%, LHV of 7.565²⁰ and boiler efficiency of 90% (steam delta H of 2.8 MJ kg⁻¹).

^BAssuming a moisture content of 50% in line with literature.

^CSteam demand for an improved industrial processing plant, reducing the steam demand from 540 to 278 kg steam TC⁻¹.⁹⁰ According to Ensinas *et al.* steam demand is 23.7 kg s⁻¹ for juice treatment, and 0.1 and 14.8 kg s⁻¹ for sugar drying and distillation respectively (500 TC h⁻¹ capacity plant).⁹⁰

^DElectricity demand based on electricity use for cane reception as specified by Dias *et al.*²⁰

^EElectricity demand ethanol dehydration is 4 MW for a dehydration unit with a capacity of 150 M year⁻¹ (13 MW for 500 ML year⁻¹).²¹ The electricity demand ranges from 0.18 to 0.33 kWh kg ethylene.^{21,93}

^FNatural gas demand (used together with fuel gas in a boiler) is 7 MW for a dehydration unit with a capacity of 150 ML year⁻¹ (24 MW for 500 ML year⁻¹).²¹

^GElectricity consumption based on the study of Alves *et al.* (2016).⁸⁸

^HElectricity use for the conversion of glycerol to 1,3-PDO is 0.1 MMBtu ton⁻¹.⁸⁷

^INatural gas input for the process described by Dunn *et al.*, is set to 13 MMBtu ton⁻¹.⁸⁷

^JSteam consumption for the production of electricity.⁸⁹

sidered, again with little variation in the energy demand. The energy consumption for the production of 1,3-PDO is based on Dunn *et al.*⁸⁷ For succinic acid, a detailed assessment is provided by Alves *et al.*,⁸⁸ which is in line with Efe *et al.*¹⁶ The variability and uncertainty of the costs and GHG emissions associated with the energy consumption was taken into account by considering the variation in price and GHG emission intensity of electricity (see below).

Economic data

Equipment and total investment costs for the different processing components

Table 4 presents an overview of the equipment costs of the individual processing steps of the different industrial processing pathways to produce ethanol, ethylene, 1,3-PDO or succinic acid. This overview includes the equipment costs, and the Lang factors applied for each processing step. For the base value, the industrial scale is set to 500 TC h⁻¹ for sugarcane, in line with Dias *et al.*,²⁰ with a scale range set to 100–1000 TC h⁻¹. Considering the Higher Heating Value (HHV) of sugarcane stalks, as described in Leal *et al.*,⁷⁰ this scale range corresponds to 138–1383 MW. For eucalyptus, the same scale (MW input) is used; this translates into a range of 7.7–77 dry tonne h⁻¹ for eucalyptus processing.

Economic data are inherently uncertain. The data for first-generation industrial production taken from Jonker *et al.*²² are in line with other studies.^{20,94,95} The equipment costs for second-generation industrial ethanol production

are moderately uncertain, as is also indicated by Chovau *et al.*⁵³ The most important variation results from the selection of technology, which also influences the BPY and investment costs. Results of economic assessments of ethanol dehydration from other studies^{17,21} are in the same range. However, uncertainty increases at larger scales and the maximum scale to which the scaling factors can be applied is uncertain. For the capital investment of ethanol and ethylene production, an uncertainty range of $\pm 25\%$ is applied, similar to Mariano *et al.*⁹⁶

The detailed published data on the total investment costs of succinic acid production was limited to Efe *et al.* and Gargalo *et al.*^{16,93} These studies agree on the BPY, but for energy consumption, capital investment cost, and operational costs, a wide range is found in these studies. This study assumed that the economic and GHG emission data for succinic acid production from sucrose are highly uncertain. Only one study was found using eucalyptus.⁸⁸ However, it is assumed that the data on succinic acid production from eucalyptus is highly uncertain. Economic data and energy consumption for 1,3-PDO production is based on studies using glycerol as feedstock,^{25,93} or studies addressing 1,4-butanediol (BDO) production.²³ The uncertainty of equipment costs and the FCI are expressed as normal distributions. The base value is considered to be the mean value of the normal distribution, with a standard deviation corresponding to 5% of the FCI for ethanol and ethylene, and 10% for 1,3-PDO and succinic acid. Such standard deviations correspond roughly to $\pm 15\%$ and 30% variation.

Table 4. Equipment costs, base scale, maximum scale, and scaling factors for the different industrial processing pathways.

Unit	Equipment	FCI (MUS\$)	Lang factor	Base capacity	Max scale	Scaling factor
Sugarcane crushing ^a	23 MUS\$	55	3	500 TC h ⁻¹	500 TC h ⁻¹	0.64
Fermentation + ethanol recovery ^a	27 MUS\$	74	3	44.5 m ³ h ⁻¹	25 m ³ h ⁻¹	0.83
Cogeneration ^a	37 MUS\$	99	3	140 dry tonne h ⁻¹	—	0.75
Ethanol – ethylene dehydration ^b	7.3 MUS\$	29	4	8764 kg ethanol h ⁻¹	—	0.65
Handling and pretreatment ligno-cellulosic biomass ^c	22 MUS\$	88	4	50 dry tonne h ⁻¹	80 dry tonne h ⁻¹	0.7
Hydrolysis ^c	4.3 MUS\$	17.2	4	50 dry tonne h ⁻¹	80 dry tonne h ⁻¹	0.6
Fermentation and 1,3 PDO recovery ^d	5.35 MUS\$	22.28	4	688 kg PDO h ⁻¹	—	0.7
Fermentation and succinic acid recovery ^e	47.11 MUS\$	183	4	5313 kg SA h ⁻¹	5500 kg SA h ⁻¹	0.7

^aFor sugarcane crushing, the study of Jonker *et al.* described in detail the equipment costs, capacity, and scale.²²

^b17,21

^c17

^d93

^eBased on the studies of Efe *et al.* and Alves *et al.*^{16,88}

Biomass feedstock supply costs and GHG emission intensity and operational costs and GHG emissions of industrial processing

Table 5 shows the supply costs and GHG emission intensity of sugarcane and eucalyptus feedstock. The operational costs and known GHG emission intensity of industrial processing are also depicted. For 1,3-PDO and succinic acid, the industrial operational costs are not known. It is assumed that the annual costs of minor operational inputs are covered by the fixed percentage of operational expenses, as discussed below.

Fossil reference

Fossil reference price

The prices of fossil reference fuels and chemicals are used to compare the selected biofuel and biobased chemicals (see Table 6). The cost ranges of fossil reference products

are determined using the crude oil price variation as basis, as discussed below.

Fossil reference GHG emission intensity

The total factory gate GHG emissions of the petrochemical products are expressed as CO_{2eq} emissions per kg product (see Table 7).

For *gasoline*, the processing GHG emissions are 12.5 g CO_{2eq} MJ_{fuel}⁻¹, and the combustion emissions are 69.3 g CO_{2eq} MJ_{fuel}⁻¹.⁹⁹ Total GHG emissions of gasoline are 81.77 g CO_{2eq} MJ_{fuel}⁻¹, which are in line with the 69.9 and 96.9 g CO_{2eq} MJ_{fuel}⁻¹ values reported by other studies.^{44,104,105} To compensate for lower energy content of ethanol compared to gasoline, a correction factor between 1.3 and 1.6 liter ethanol liter⁻¹ conventional gasoline is applied, depending on the car engine and percentage ethanol in the gasoline-ethanol fuel mix. The higher heating value of gasoline is based on a study by Faaij.¹⁰³

Table 5. Feedstock supply and industrial operation costs and GHG emissions.

Item	Unit	Value	Range	Reference
Sugarcane cultivation	US\$ TC ⁻¹	31 ^a	Normal distribution, st. dev. 0.45	81, ⁹⁶
	kg CO _{2eq} TC ⁻¹	26 ^b	Uniform; min. 29.6, max. 35.5	
Sugarcane transport	US\$ TC ⁻¹	6 ^c	—	22, ⁶⁰
	kg CO _{2eq} TC ⁻¹	2.45 ^d	—	60
Eucalyptus supply	US\$ tonne ⁻¹	48 ^e	Normal distribution, st. dev. 0.91	60
	kg CO _{2eq} tonne ⁻¹	22.45 ^f	Uniform; min. 19.1, max. 25.8	60
Electricity	US\$ MWh ⁻¹	61	Uniform; min. 42, max. 80	96
	kg CO _{2eq} kWh ⁻¹	0.094 ^g	Uniform, min. 0.025, max. 0.65	97, ⁹⁸
Annual maintenance expenses	% of FCI	2	—	21
Annual labor expenses		3	—	21
Annual operational expenses		0.75	—	68
Operational hours first generation	Hours	4080 ^h	—	22
Operational hours second generation		8000	—	84

^aThe average sugarcane price between 2001 and 2011 is 26 US\$₂₀₁₁/tonne.⁸² For today we consider a value of 30 US\$/tonne, based on Jonker *et al.* (2015) and Mariano *et al.* (2013)^{22,96}

^bSugarcane cultivation, excluding trash burning and cane transportation, values for 2005–2006 season.⁹⁹

^cConsidering an average distance between field and industrial plant of 30 km and truck transport, as specified in Jonker *et al.*⁶⁰

^dSugarcane transport, using distance (23 km), truck fuel efficiency (0.019 L t⁻¹ km), and diesel GHG emission intensity of 3.87 kg CO_{2eq} L⁻¹.^{60,99}

^eAlthough there is currently no market for sugarcane trash, in this analysis a potential price is included, based on the studies of Jonker *et al.*, mainly referring to industry experts.⁶⁰

^fAssuming the same GHG emission intensity for trash transport (wet) as wet sugarcane stalks, see above.

^gThe emission intensity of the electricity mix in Brazil is relatively low due to the high contribution of hydropower and also the use of bagasse for the production of bioelectricity. Due to the seasonality of these technologies, the GHG emission intensity of the electricity mix in Brazil varies inter and intra annually. We therefore consider a broad range of GHG emission intensity for electricity replaced in Brazil. The lower end of the range is based on the lowest emission intensity of Brazilian electricity mix in the past decade reported by the Ministry of Science, Technology, Innovation and Communication.⁹⁸ The high end of the range represents the emission intensity of a gas fired power plant in Brazil.⁹⁷ The average emission intensity is based on the Brazil specific values reported by McKinsey¹⁰⁰ and the World Energy Outlook of the IEA⁵

^hFor integrated first- and second-generation ethanol production we also assume an operating time of 4080 hours for the entire plant.²²

Table 6. Price of fossil reference products and Brazilian electricity.

Item	Base value US\$ kg ⁻¹	Range ^a US\$ kg ⁻¹
Gasoline fuel fossil reference	0.55 ^b	0.44–1.42
Ethylene fossil reference	1.2 ^c	0.78–1.62
1,3-PDO	2.02 ^d	1.24–2.80
Succinic acid	2.5 ^e	1.54–3.46

^aUsing the crude oil price variation of the last 10 years as proxy for the price variation, and the price increase factors of 0.77, and 0.96 for electricity and petroleum products respectively.

^bAssuming the costs of crude oil and refining are similar in different parts of the world. Using the approach of Van Vliet *et al.* (2009)¹⁰¹ to calculate the production costs of gasoline based on the crude oil price: a price mark-up of 30% for refining is used. An oil price range of 40 to 130 US\$ bbl⁻¹,²¹ is used, with 50 US\$ bbl⁻¹ as current price.¹⁰² The costs for taxes and distribution are not included. The costs shown here are per kg fossil product; however, to account for the difference in energy content, the fuel characteristics of ethanol (density 0.79 kg L⁻¹, 30 MJ kg⁻¹) and gasoline (0.75 kg L⁻¹, 46 MJ kg⁻¹ are used).¹⁰³

^cThe price variation of the ethylene market price varied between 2006 and 2012 in a range of 719–1850 US\$ tonne⁻¹ (oil price variation between 40 and 130 US\$ bbl⁻¹).²¹

^dAverage price for 1,3-PDO in US\$ kg⁻¹ is based on the study of Gargalo.¹⁰² A standard deviation of 0.35 is considered.

^eAccording to Weastra *et al.*⁵⁷ the price of petrol based succinic acid varies between \$2.4–2.6 kg⁻¹ depending on the purity and quality of the succinic acid. (110) reported the production costs of maleic anhydride-based succinic acid as 2.554 € kg⁻¹. Biobased succinic acid is slightly more expensive (\$2860–3000 metric tonne⁻¹).¹²³ Average price for succinic acid in US\$ kg⁻¹, with a standard deviation of 0.23⁹³.

Table 7. Greenhouse gas emissions of fossil reference chemicals.

Item	Total GHG emissions	Unit	Reference
Gasoline	1.52–2.59	kg CO _{2eq} L ⁻¹ ethanol equivalent	44,104,105
Ethylene	3.8–4.89	kg CO _{2eq} kg ⁻¹	106–110
1,3-PDO	4.04–9.4	kg CO _{2eq} kg ⁻¹	72,73,109
Succinic acid	3.43–8.59	kg CO _{2eq} kg ⁻¹	109,111

Reported values for GHG emissions of ethylene production are between 710 and 1800 g CO_{2eq} kg⁻¹ ethylene.^{106–110} For ethylene production, the GHG emissions are dominated by the energy (fuel and electricity) consumption, mainly in the steam cracker.^{107,110} The embedded carbon in ethylene is equal to 3.09 kg CO_{2eq} kg⁻¹ ethylene (based on C-content of 84.3%), in line with data reported by McKechnie *et al.*¹⁰⁶

Different production pathways exist for the production of fossil 1,3-PDO. Hydroformylation of ethylene

oxide is the dominant pathway.¹¹² For this analysis, the carbon embedded in PDO (based on chemical structure) is considered being equivalent to 1.736 kg CO_{2eq} kg⁻¹ PDO. A literature review found four studies reporting on the GHG emission intensity of factory-gate fossil PDO.^{72–74,109} By adding the embedded CO_{2eq} to the results presented in the study of Patel *et al.*,¹⁰⁹ the total GHG emission intensity of all studies is in the range of 4.04–9.4 kg CO_{2eq} kg⁻¹ PDO.^{72–74,109} The upper level of this range is found in Urban and Bakshi,⁷³ using a process LCA for a production facility in Louisiana, USA. Using the same geographic location but a hybrid LCA approach, the GHG emission intensity of fossil PDO would decrease to 6.7 kg CO_{2eq} kg⁻¹ PDO.⁷³ As it is not clear if this upper level includes the embedded carbon, which is potentially emitted to the atmosphere as CO₂, this level can even increase to 11.14, which is in line with data presented by Dunn *et al.*⁸⁷

The number of studies presenting the GHG emission intensity of succinic acid is limited. Succinic acid is mainly produced by the hydrogenation of maleic acid, which is produced by the oxidation of benzene or butane.¹¹³ Only two studies were found on the GHG emission intensity. Of these, one presented the cradle-to-grave GHG emissions. By including the embedded CO_{2eq} in succinic acid, the GHG emission range found is between 3.43 and 8.59 kg CO_{2eq} kg⁻¹ succinic acid.^{109,111} Considering the potential derivatives for succinic acid, maleic anhydride can also be considered as fossil reference, which has a GHG emission intensity of 3.58–6.80 kg CO_{2eq} kg⁻¹ succinic acid.^{109,111} For both products, the large non-renewable energy consumption (32.7 and 60.8 MJ kg⁻¹ succinic acid and maleic anhydride respectively) dominates the GHG emissions.¹¹¹

Results

This section compares the techno-economic and GHG emissions intensity performances of the four biobased products (i.e. ethanol, ethylene, 1,3-PDO, and succinic acid) using sugarcane and eucalyptus as feedstocks in the Brazilian context. This comparison not only allows the most promising products (from an economic and environmental perspective) to be identified but also potential synergies between these two feedstocks to develop biobased products more effectively, as these two crops are major products from different regions – sugarcane is mainly cultivated in São Paulo state¹¹⁴ whereas eucalyptus is mainly grown in the states of Minas Gerais and Rio Grande do Sul.¹¹⁵

Techno-economic results of the industrial processing pathways

Table 8 shows the FCI, biobased product yield (BPY), electricity surplus, and the biobased product cost (BPC) for the selected sugarcane and eucalyptus processing pathways. Both the BPY and the BPC are shown for a 90% confidence interval. The steam production in the cogeneration unit is based on the amount of sugarcane bagasse or eucalyptus residues and results in 0.62 tonne steam TC⁻¹ and 2.6 tonne steam dry tonne⁻¹ eucalyptus. When sugarcane bagasse is utilized for ethanol production, the steam production is reduced to 0.40 tonne steam TC⁻¹. The steam production is used for process steam demand and for electricity production. The electricity that is produced is used to meet the process electricity demand and the surplus electricity is sold to the grid. The uncertainty range for BPY and BPC for first-generation ethanol from sugarcane is smaller than the uncertainty range for first- and second-generation ethanol. This is the result of the relatively large uncertainty ranges in sugarcane feedstock cost and sucrose content, which play a more prominent role in first-generation ethanol production. Given the high glucan content, the BPYs of the eucalyptus production pathways are higher compared to the sugarcane pathways. However, the BPCs for ethanol, ethylene and 1,3-PDO are higher for the production pathways using eucalyptus compared to the pathways using sugarcane. Due to the greater uncertainty of the conversion efficiencies, the BPY ranges of 1,3-PDO and succinic acid production are larger compared to ethanol and ethylene production. The higher FCIs for the production pathways of 1,3-PDO and succinic acid are predominantly caused by the high equipment costs of the product recovery and purification. The high FCI for succinic acid

production of sugarcane compared to that of eucalyptus is the result of the larger scale of the succinic acid processing pathway of sugarcane and the limited economies of scale.

Biobased production costs breakdown

The contribution of the different cost components to the production costs of the different industrial pathways for the production of ethanol, ethylene, 1,3-PDO and succinic acid is shown in Fig. 2. The main cost elements of the total biobased production costs are biomass feedstock, capital investment, energy (as co-product or as net energy consumption), and the processing inputs. The contribution of feedstock costs decrease with increasing biobased product yield (BPY). For example, the high glucan content and high conversion efficiency result in a low share of feedstock costs for succinic acid production using eucalyptus. Compared to ethanol production, the other industrial pathways have a high contribution from capital depreciation to the total costs. The contribution of capital cost are especially high for succinic acid production from sugarcane. This is due to the limited operating hours of the plant and related limited annual output, which results in a high capital cost per unit of output. For eucalyptus-processing pathways, the costs associated with enzymes for pretreatment and hydrolysis result in a large contribution of processing inputs to the total production costs, compared to the pathways using sugarcane. The fermentation and purification of 1,3-PDO and succinic acid require a significant amount of steam and electricity. The high energy demand is partly covered by the use of bagasse from sugarcane or the residues from eucalyptus (mainly lignin). However, as that is not sufficient to meet the total process energy demand, externally purchased energy contributes significantly to the total costs.

Table 8. Ranges of biobased product yield, biobased production costs, fixed-capital investment base value, and electricity surplus for the different industrial processing pathways.

Feedstock	Biobased product	BPY range 90% (Kg biobased product tonne ⁻¹ biomass)	Annual production (Mtonne year ⁻¹)	Fixed capital investment base value (MUS\$)	Electricity surplus (kWh tonne ⁻¹ biomass)	BPC 90% US\$ kg ⁻¹ biobased product
Sugarcane	Ethanol 1G	57–72	131	245	67	0.60–0.83
Sugarcane	Ethanol 1+ 2G	79–96	185	322	–44	0.60–0.77
Eucalyptus	Ethanol 2G	204–268	75	174	100	0.83–1.23
Sugarcane	Ethylene	34–43	76	300	41	1.10–1.57
Eucalyptus	Ethylene	122–161	43	203	–5	1.64–2.23
Sugarcane	1,3-PDO	54–78	126	692	–242	1.25–1.74
Eucalyptus	1,3-PDO	160–241	64	271	–1211	1.72–2.73
Sugarcane	Succinic acid	71–135	218	1995	–585	1.68–3.40
Eucalyptus	Succinic acid	215–415	51	565	–2250	1.56–3.15

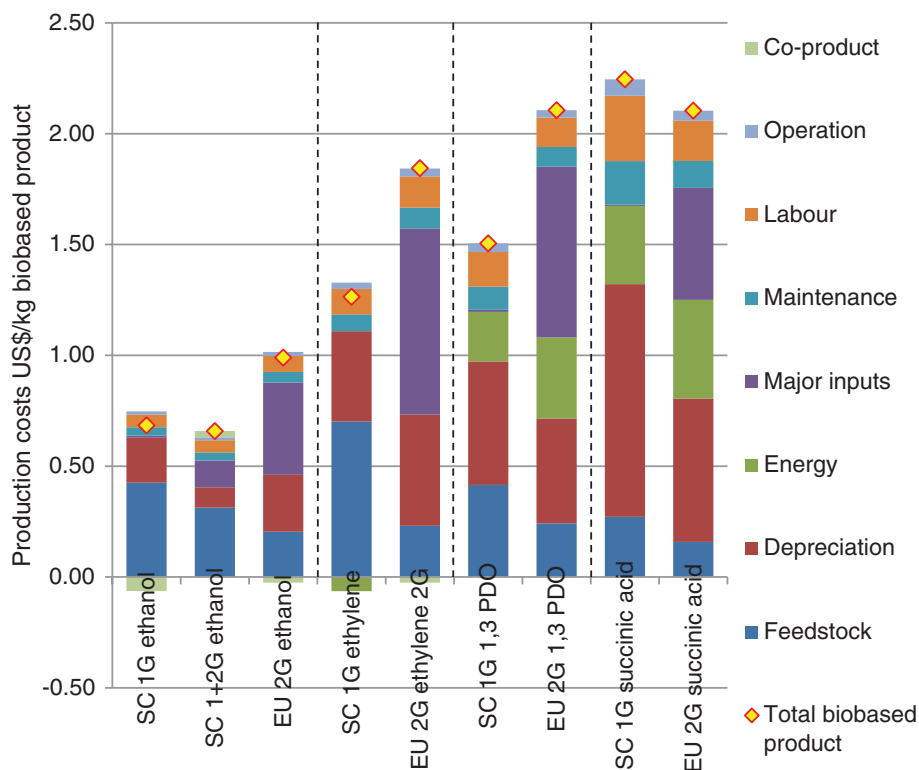


Figure 2. Contribution to the production costs of ethanol, ethylene, 1,3-PDO and succinic acid production using sugarcane and eucalyptus feedstock.

Sensitivity analysis for key economic parameters

A sensitivity analysis is performed to analyze the effect of the uncertainties in BPY, feedstock costs, total investment costs, scaling, and the energy price, on the total production costs and GHG emission intensity. The results are plotted in various spider diagrams (see supplementary information SI.3, File S1). The variation in BPY has the largest impact on the production costs as this affects the annual product output and in that way impacts the production costs per unit of output. However, only the production of 1,3-PDO and succinic acid have a potentially large range in BPY. After the BPY, the production costs for first-generation ethanol, first- and second-generation ethanol, and sugarcane ethylene are most impacted by the sugarcane feedstock costs. Second-generation ethanol and ethylene from eucalyptus are more affected by the investment costs. For 1,3-PDO and succinic acid, the patterns of sensitivity for the uncertainty in input parameters are similar for the processing pathways from sugarcane and eucalyptus and are mostly impacted by the variation in the FCI and electricity price.

Range of biobased production costs

The ranges of the production costs of the biobased products and of the prices of the petrochemical equivalent products are shown in Fig. 3. Within the ranges of the biobased product costs, the mean production costs and the production cost ranges for the 90%, 80%, and 60% confidence intervals are distinguished. The different levels of probability show the robustness of the results according to the uncertainty ranges in the input data. The more complex biobased production pathways have a larger uncertainty range in the production costs compared to ethanol and ethylene, because of the higher uncertainties in the BPY and investment cost and due to a relatively large contribution of highly uncertain energy costs.

The production cost of ethanol is in the range of 0.64–1.10 US\$ kg⁻¹ ethanol (60% confidence) for first-generation, integrated first- and second-generation, and second-generation industrial processing of sugarcane and eucalyptus. This cost range is mostly higher than the range in factory gate gasoline prices (0.29–0.92 US\$ kg⁻¹ ethanol equivalent). The cost of biobased ethanol is in the same range as gasoline in case of high crude oil prices (130 US\$ bbl⁻¹) and when biomass feedstock costs and total capital

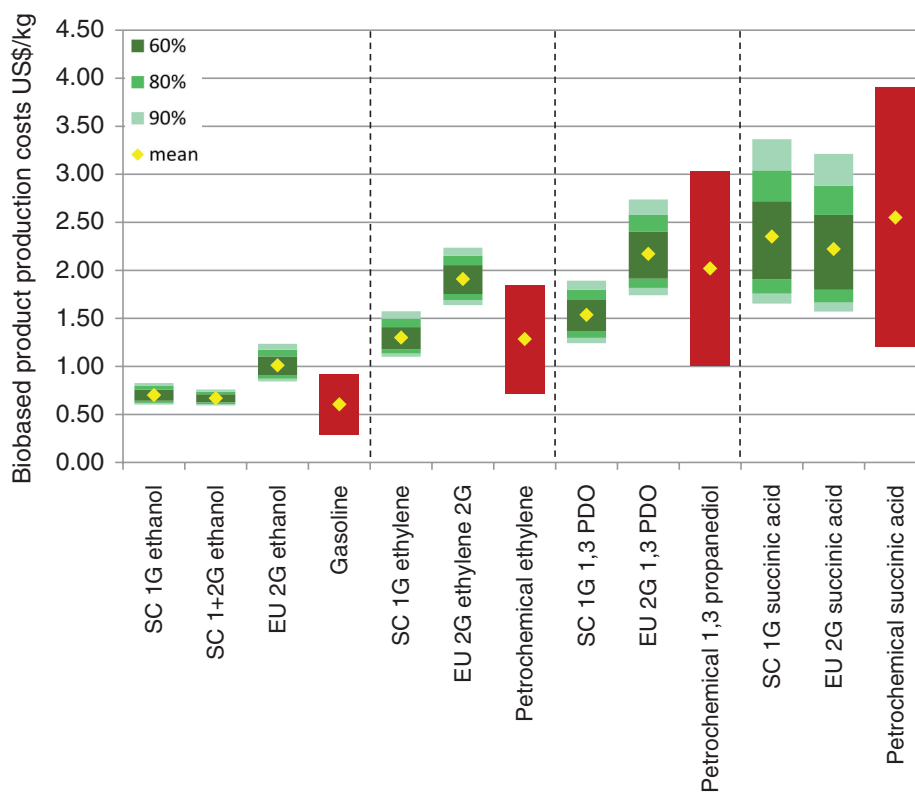


Figure 3. Uncertainty ranges of production costs of the different biobased products and their respective fossil references.

investment costs are at the lower end of the indicated ranges. The cost range of ethanol found in this study only partly overlaps with the range of ethanol producer prices (0.49–0.69 US\$ kg⁻¹ ethanol) of the past 3 years in Sao Paulo state reported by UNICA.¹¹⁶ The ethylene production costs found in this study are in the range of 1.18–2.05 US\$ kg⁻¹ ethylene. In comparison, the fossil ethylene production price range is 0.72–1.85 US\$ kg⁻¹ ethylene. As the BPY of ethylene is lower compared to ethanol and the additional dehydration unit requires more capital investment and a larger amount of process energy, the ethylene production costs are almost twice as high compared to ethanol production costs. For 1,3-PDO, the biobased production costs are in the range of 1.37–2.40 US\$ kg⁻¹ PDO, which is well within the range of the calculated petrochemical PDO price. The base value of production costs of biobased PDO using sugarcane is also lower than the base value of petrochemical PDO. Similar to PDO, the biobased production costs of succinic acid using sugarcane and eucalyptus are between 1.91 and 2.57 US\$ kg⁻¹ succinic acid. This is within the range of the petrochemical succinic acid prices. More importantly, the base value costs are lower compared to the base value costs of petrochemical

succinic acid. Due to the greater uncertainty in BPY, FCI, and energy consumption (and their impact on total production costs) the confidence ranges of 60%, 80%, and 90% are larger for 1,3-PDO and succinic acid compared to the ranges for ethanol and ethylene.

The estimated biobased production costs of succinic acid are lower for the pathway using eucalyptus compared to the pathway using sugarcane, due to lower investment costs. On the other hand, sugarcane is more convenient for ethanol, ethylene, and 1,3-PDO production due to efficient processing (little need for costly inputs like enzymes) and low investment costs.

GHG emission breakdown

The mass and energy inventory was used to determine the biobased product yield and the GHG emissions, expressed in kg CO_{2eq} per kg biobased product at the factory gate (see Fig. 4). Greenhouse gas emissions include the emissions related to feedstock supply, industrial processing and the emissions associated with the additional steam, heat, and electricity demand. For the processing of sugarcane to ethanol, eucalyptus, to ethanol, and sugarcane to ethylene,

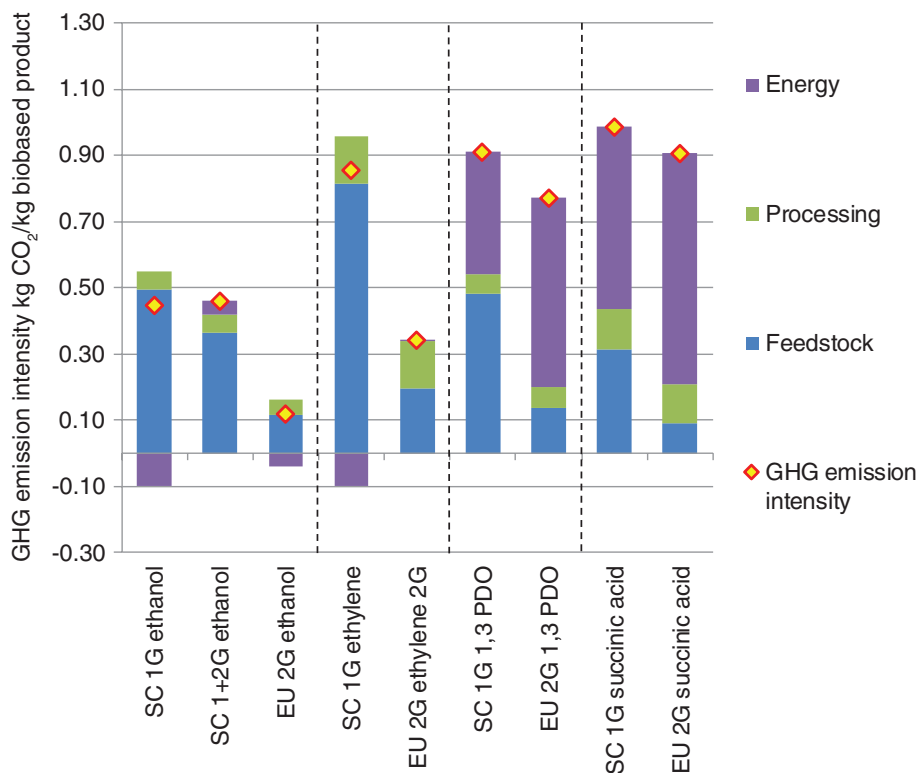


Figure 4. Contribution to the GHG emission intensity of ethanol, ethylene, 1,3-PDO, and succinic acid production using sugarcane and eucalyptus feedstock.

the electricity surplus results in negative emissions due to the electricity surplus. Similar to the economic performance, the contribution from the cultivation stage to the overall GHG emissions are reduced with higher biobased product yield. For the production of 1,3-PDO and succinic acid, the high steam and electricity demand (not covered by the cogeneration unit) result in a large amount of GHG emissions. For all biobased products, the production pathways using eucalyptus as feedstock have a lower GHG emission intensity compared to the pathways using sugarcane, due to the lower GHG emissions associated with the feedstock production.

Sensitivity analysis for key GHG emission intensity parameters

The results of the sensitivity analysis for the GHG emission intensities, varying the feedstock GHG emission intensity, BPY, and electricity GHG emission intensity, are shown in the supporting information, SI.2, File S1. For the biobased products whose GHG emission intensity is caused mainly by the feedstock supply GHG emissions, a change of the GHG emission intensity of feedstock supply or the BPY has the largest influence on the total GHG

emission intensity. Examples are the sugarcane to ethanol (first-generation industrial technology) and sugarcane to ethylene production pathways (see Fig. 4) and supporting information SI.2, File S1. For industrial pathways for which the GHG emission intensity is mainly caused by the energy demand, the total GHG emission intensity varies strongly with a variation in the GHG emission intensity of process energy. In general, the sensitivity in GHG intensity of the biobased products shows similar patterns for the pathways based on eucalyptus feedstock and the pathways using sugarcane feedstock. Only for 1,3-PDO and succinic acid is the GHG intensity of the sugarcane pathways slightly more sensitive to variations in the feedstock-related GHG emissions compared to the pathways using eucalyptus.

Range of GHG emission intensity

The uncertainty ranges of the GHG emissions associated with the production of biobased chemicals are shown in Fig. 5 together with the range of the GHG emission intensity of fossil gasoline, ethylene, 1,3-PDO and succinic acid equivalent products. For the 1,3-PDO and succinic acid based on sugarcane and eucalyptus, the large range

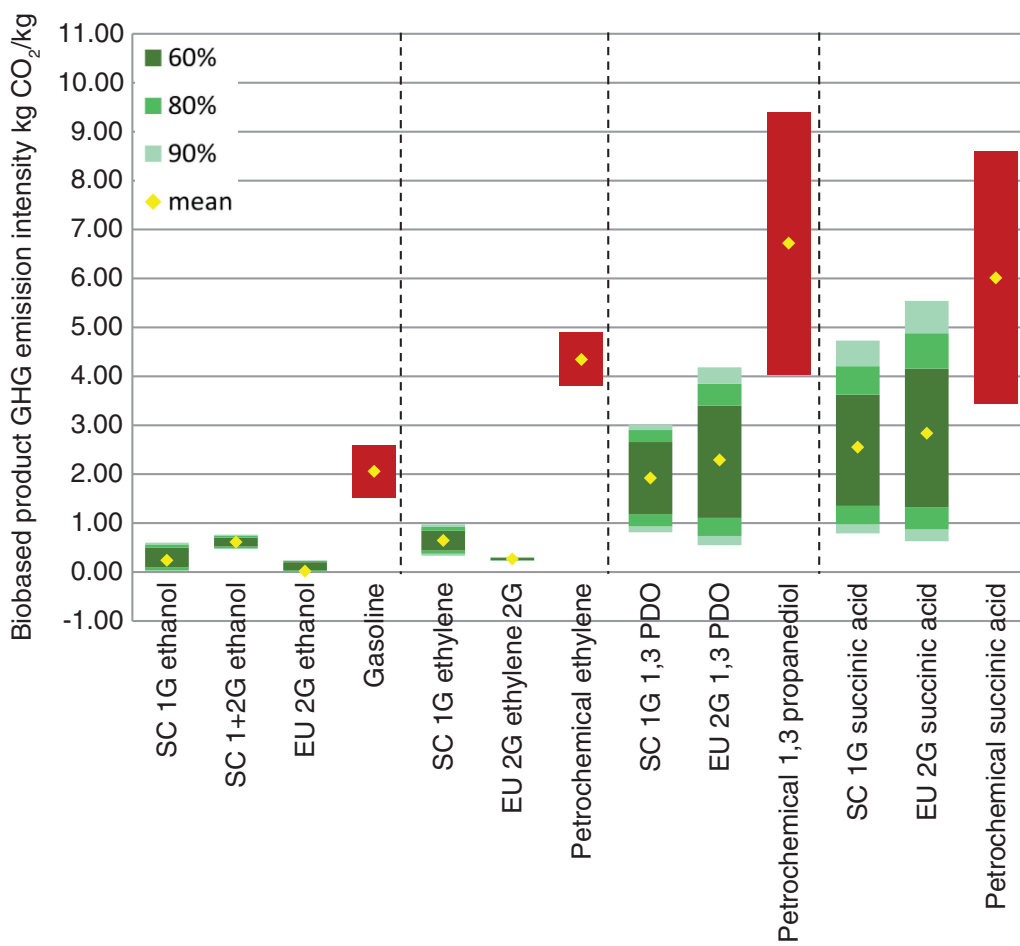


Figure 5. Uncertainty range of the GHG emission intensity of the different biobased products and their respective fossil references.

is mainly caused by uncertainty in the GHG emission intensity of electricity. For ethanol and ethylene, the GHG emissions intensity may even be negative due to the credited GHG emissions of electricity surplus. Overall, the range of GHG emission intensities of the biobased chemicals is lower than the range of the petrochemical reference.

The GHG emission intensity of ethanol production using sugarcane or eucalyptus feedstock is in the range of -0.06 – 0.76 kg CO_{2eq} kg⁻¹ ethanol. The low values are the results of low GHG emission for biomass supply, high BPY, and credited electricity surplus GHG emissions. Similarly, for ethylene production, the credited GHG emissions result in low GHG emission intensities (0.23 – 0.98 kg CO_{2eq} kg⁻¹ ethylene) compared to the petrochemical reference. Note that a large fraction of the GHG emissions of petrochemicals is due to the embedded fossil carbon released during the combustion. For both ethanol and ethylene, the use of eucalyptus results in lower GHG emissions than sugarcane due to the large

amount of residue available for electricity production. For 1,3-PDO and succinic acid, the upper level of the GHG emission intensity range overlaps with the lower end of the GHG emission intensity of the petrochemical equivalent. Biobased 1,3-PDO and succinic acid have a GHG emission intensity in the range of 0.55 – 4.18 kg CO_{2eq} kg⁻¹ PDO and 0.63 – 5.54 kg CO_{2eq} kg⁻¹ succinic acid respectively. These values are due to the high energy consumption for recovery and purification. This high energy demand cannot be covered fully with the processes' own production of steam and electricity and therefore requires the supply of electricity from the grid.

Potential profit margin and GHG emission reduction per hectare cultivation area

Figure 6 depicts the potential net profit and net GHG emission reduction by the use of sugarcane and eucalyptus for biobased products in Brazil, expressed in US\$ ha-year⁻¹

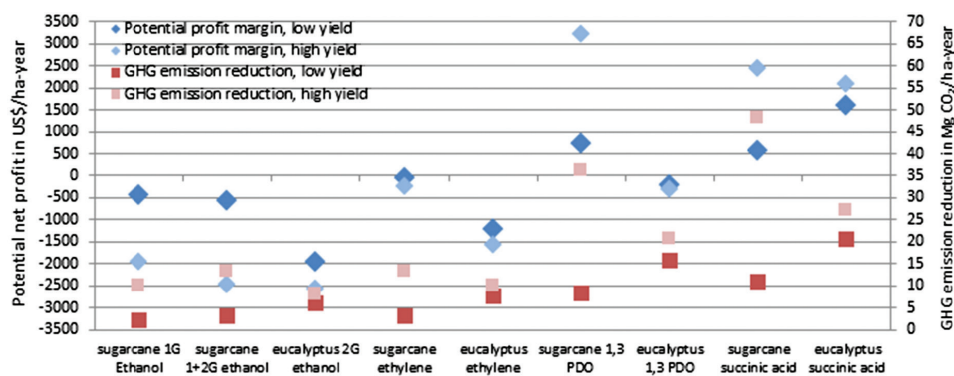


Figure 6. Potential net profit and GHG emission reduction per hectare of cultivation area for the different biobased production pathways.

and $\text{Mg CO}_{2\text{eq}} \text{ ha-year}^{-1}$ for a low and high biomass yield scenario. Figure 6 only shows the base values for potential net profit and net GHG emission reduction for these two yield scenarios. In the low-yield scenarios, the eucalyptus pathways have a higher GHG emission reduction than the sugarcane pathways. However, in the high-yield scenarios, the pathways using sugarcane realize more GHG emission reduction. From an economic point of view, the sugarcane pathways also score better than eucalyptus.

All biomass production pathways result in a net GHG emission reduction per hectare, varying between 2 to 21 and 8 to 48 $\text{Mg CO}_{2\text{eq}} \text{ ha-year}^{-1}$ for the low- and high-yield scenarios respectively. At an oil price of $50 \text{ US\$ bbl}^{-1}$, the ethanol and ethylene production pathways have difficulty to compete with the fossil products price, while the production of 1,3-PDO and succinic acid production from sugarcane and the production of succinic acid based on eucalyptus can be profitable. However, the uncertainties in the economic performance and GHG emission intensities, as discussed above, are not considered in this figure.

Discussion

In this study, the costs and GHG-emission intensity of ethanol, ethylene, 1,3-PDO, and succinic acid production from sugarcane and eucalyptus are quantified and compared with the fossil-equivalent product. A uniform approach is applied to quantify the uncertainty ranges in the production cost (Fig. 3) and GHG emission intensity (Fig. 5) of the different biobased production pathways. This uniform approach allows for a harmonized and fair comparison of the production cost and GHG emission performance of the four selected products and the industrial pathways. This approach also allows for the identification of the major contributors to the production costs and GHG emissions in a transparent manner. The tradeoffs

between the economic and GHG emission performance can also be assessed, which enables the selection of the best performing routes in a transparent manner.

The current analysis does not include the potential integration or co-production of the selected biobased industrial processing pathways. The considered input values for the GHG emission intensity and costs of electricity and biomass feedstock are based on the current situation. However, with increasing demand, the parameters determining the economic and GHG performance are likely to change in the future and may affect the ranking of best performing pathways.

The results should be interpreted as ranges rather than single values, given the uncertainties in the costs and GHG emission intensity of biomass supply, biobased product yield, total capital investment, and costs and GHG emission intensity of energy. The cost and GHG emission ranges are based on the considered ranges and the probability distributions for BPY, biomass feedstock supply, industrial scale, FCI, and GHG emission intensity, and price and GHG emission intensity of process energy demand. For 1,3-PDO and succinic acid production, the estimated uncertainty is higher than for ethanol and ethylene, due to the limited data availability. The assumptions on the uncertainty range of the different parameters have a higher impact on the range of the final results than the choice of probability distribution of the parameter. In this analysis, considerable attention is therefore given to the selected range of the BPY, as it is a key parameter in the quantification of both the production costs and GHG emission intensity of the biobased products. As shown in Table 9, the (calculated) BPYs of all conversion processes considered in this study are in line with the ranges found in literature.

The production cost ranges for the biobased chemicals investigated in this study partly overlap with the calculated ranges of production prices of the petrochemical

Table 9. comparison of the BPY of various conversion routes used in this study with values found in the literature.

Conversion routes	Unit	BPY found this study	BPY found in literature	References
First-generation ethanol using sugarcane	kg EtOH TC ⁻¹	57–72	60–102	20,22,69
Integrated first- and second-generation ethanol using sugarcane	kg EtOH TC ⁻¹	79–96	78–90	95
Second-generation ethanol using eucalyptus	kg EtOH tonne ⁻¹ EU	204–268	196–297	95
Ethanol to ethylene conversion	kg ETE kg ⁻¹ EtOH	0.598	0.572–0.609 ^a	21,52,107
Production of 1,3-PDO from sugars	kg PDO kg ⁻¹ sugars	0.46	0.44	88
Production of succinic acid from sugars	kg SA kg ⁻¹ sugar	0.78	0.61–0.92 ^a	88

^aThe upper end of this range represents a mass conversion efficiency of 94–99%.

Table 10. Greenhouse gas emission reduction potential of ethanol, ethylene, 1,3-PDO and succinic acid. Expressed in absolute numbers, in five compared to the fossil reference and in per cultivated area.

Biobased product	Results of this study			Found in literature	
	Absolute kg CO _{2eq} kg ⁻¹ biobased product	Relative % compared to fossil reference	Per area Mg CO _{2eq} ha-year ⁻¹	Absolute kg CO _{2eq} kg ⁻¹ biobased product	Relative % compared to fossil reference
Ethanol	1.3–2.2	63–105	2–13	2.6–3.0 ^{a,b,c}	123–143 ^{a,b,c}
Ethylene	3.4–4.1	78–95	3–13	0.6–3.4 ^{a,b,c}	14–78 ^{a,b,c}
1,3-PDO	2.5–5.9	38–88	8–36	2.8–6.7 ^{a,b}	42–99 ^{a,b}
Succinic acid	0.5–5.2	8–87	11–48	2.7–5.5 ^{a,b}	46–92 ^{a,b}

^aValues taken from and calculated based on the data reported by de Jong *et al.*¹¹⁸

^bValues taken from and calculated based on the data reported by Montazeri *et al.*¹¹⁹

^cValues taken from and calculated based on the data reported by Posen *et al.*^{120,121}

equivalent products. The base values for the biobased products, as reported in Fig. 3, are in some cases higher (ethanol, ethylene and 1,3-PDO from eucalyptus) and in other cases lower (1,3-PDO from sugarcane and succinic acid) than the fossil-equivalent products but the differences are small. With current oil prices of 50 US\$ bbl⁻¹, most of the biobased production pathways have difficulty to compete, but increasing oil prices can increase the economic viability. It should be noted that the effect of the oil price on the production cost of the biobased products has not been taken into account. When oil prices increase, some cost components of the biobased products are also likely to increase. Moreover, the economic assessment in this study does not consider the possible impact of taxes, tax exemptions, or premiums paid for biobased products.

As indicated by Nitzsche *et al.*, the premium of biobased ethylene can be as high as 30–60% of the price of fossil ethylene.¹⁷ The market price of more complex chemicals also depends to a great extent on the purity of the product.¹¹⁷ All of these factors complicate the assessment of the economic viability of biobased products. As the differences in the production costs between biobased and petrochemical production are small, a variation in either one can

greatly change the project's viability. As shown in Fig. 3, the fossil reference prices can vary significantly. Over the past 10 years, the crude oil price varied between 35 and 140 US\$ bbl⁻¹.²¹ For gasoline, this would correspond to an ethanol-equivalent price between 0.25 and 1.00 US\$ kg⁻¹. Such fluctuations strongly affect the profitability of biofuels and biochemicals. The potential profit margin used in Fig. 6, is based on the base values (crude oil price about 50 US\$ bbl⁻¹) of the economic quantification. An increasing oil price can therefore result in a positive potential net profit for ethanol and ethylene. For example, the largest profit margin is for sugarcane ethylene production and is 0.4 US\$ kg⁻¹. This would imply a potential net profit of 1326 US\$ ha⁻¹. On the other hand, the largest negative difference for the production of sugarcane 1,3-PDO is –0.8 US\$ kg⁻¹ product. This could mean a potential loss of –4420 US\$ ha⁻¹. When expressing the economic performance per hectare, the BPY and biomass yield ranges amplify the difference between the production costs of biobased and petrochemical products. The economic and GHG performance per hectare are strongly related to the biomass yield. Given the potential yield improvement of both eucalyptus as sugarcane, this performance may

improve significantly in the future. The use of energy cane could also potentially improve the GHG and economic performance per hectare.

The GHG emission intensities of the four biobased products considered in this study are lower than those of the equivalent fossil products. Table 10 shows the GHG emissions reduction ranges of each of these four biobased products, expressed as absolute GHG emission reduction (in kg CO_{2eq} per kg biobased product), as relative emission reduction compared to the fossil reference (%), and as GHG emissions reduction per cultivated area (in Mg CO_{2eq} ha-year⁻¹). The highest GHG emission reductions compared to the fossil based reference can be achieved by ethanol and ethylene production (i.e. approximately 60–100%). However, when the absolute GHG emission reductions are considered, the highest reductions can be achieved by 1,3-PDO and succinic acid production (i.e. up to 7.9 and 6.8 kg CO_{2eq} kg⁻¹ biobased product respectively). When results are expressed per hectare of cultivated area per year, the highest GHG emissions reduction can be achieved for succinic acid production using sugarcane as a feedstock (i.e. up to 41 Mg CO_{2eq} ha-year⁻¹). These results illustrate the fact that different choices for metrics result in different rankings of the selected industrial pathways.

The GHG emissions intensity of the biobased production pathways and their potential emissions reduction have also been compared to the LCA data of biobased products reported in the literature, as shown in Table 10. The GHG emission intensity ranges of 1,3-PDO and succinic acid estimated in this study are consistent with the values reported by de Jong *et al.*¹¹⁸ who performed a meta-analysis on the LCA data of 34 priority biobased chemicals reported in 86 discrete LCA case studies. However, in the case of ethanol, the range of GHG emission reduction estimated in this study is more conservative, whereas for ethylene production the estimated range is more optimistic compared to the range reported by de Jong *et al.* The differences with the data reported in literature are most likely due to three main reasons: (i) the raw materials used (i.e. estimations made in this study for ethylene production consider a sugarcane-based product while the other studies considered corn- and switchgrass-based products), (ii) use of different GHG emission intensities or credits for electricity or heat consumption, and (iii) use of other regional or case-study-specific data. Literature data included in Table 10 refer either to a deterministic model with a particular set of conditions,^{118,119} or to the mean values of the combination of deterministic and stochastic models.¹²⁰

A methodological challenge is the fact that there is no commonly agreed method to quantify the GHG emission intensity for chemicals such as PDO or succinic acid. For gasoline, the fossil reference is well known and defined to determine the GHG emission reduction of biofuels for transport.^{63,122} However, for chemicals from fossil feedstock no commonly agreed methods to determine reference values exist, despite the fact that these chemicals have typically already been produced for years. The range of potential fossil GHG emissions adds another source of uncertainty regarding the potential emission reduction of biobased chemicals.

Finally, it is important to note that for the calculation of the GHG emission reduction per hectare, no land-use change-related GHG emissions were taken into account in this study. Based on the study by Jonker *et al.*,⁶⁰ direct land-use change GHG emissions in the state of Goiás can be as high as 462 kg CO_{2eq} TC⁻¹ and 1571 kg CO_{2eq} tonne⁻¹ eucalyptus. This could potentially mean additional GHG emissions as high as 3.8 and 4.0 kg CO_{2eq} kg⁻¹ succinic acid for sugarcane and eucalyptus respectively, using the high-end BPY for succinic acid production as shown in Table 8. Such high direct land-use change GHG emissions can cut the GHG emission reduction potential completely. However, land-use change GHG emissions per tonne of biomass feedstock can also be zero or positive, and should therefore be included in future assessments. Similarly, indirect land-use change GHG emissions can also have a negative or positive impact, or no impact, on the GHG emission intensity per hectare.

Conclusions

The aim of this study was to quantify the production costs and GHG emission intensity of ethanol, ethylene, 1,3-PDO and succinic acid from sugarcane and eucalyptus feedstock. This enabled biobased products to be compared with their fossil equivalent products and also enabled different biobased industrial processing pathways to be compared. Due to the uncertainty associated with biobased products the results are presented in ranges. This analysis shows that sugarcane based 1,3-PDO, and, to a lesser extent, the production of succinic acid, were most economically viable. However, the costs of these production pathways are more uncertain than ethanol and ethylene production. As the differences between the biobased production costs and fossil equivalent product costs are small, the net profit, expressed per kg product or per hectare of cultivation area is very sensitive for these uncertainties. With an increasing

oil price, more biobased production pathways can become economically viable in the future.

The GHG emissions of petrochemical ethanol and ethylene are largely due to the embedded carbon in fossil-equivalent products. Apart from ethylene, the GHG emission intensity of fossil reference products depends on the GHG emissions in the supply chain, especially the emissions related to the process energy demand. Considering the potential GHG emission reduction and profit per hectare, industrial processing pathways utilizing sugarcane scored better than the pathways using eucalyptus feedstock due to the high yield of sugarcane specifically in Brazil. It was not possible to choose a clear winner, as (a) the best performing product strongly depended on the chosen metric (percentage GHG emission reduction, absolute GHG emission reduction per kg biobased product, or GHG emission reduction per hectare of cultivated land), and (b) the large uncertainty ranges found, especially for PDO and succinic acid, independent of the metric.

As indicated, the BPY, FCI, and energy consumption of different biobased production pathways are important for economic and GHG emission performance. However, these key variables are not always well documented for all of the steps of each industrial pathway. Key topics calling for further research are therefore: First, quantification of the conversion efficiencies of large-scale industrial processing facilities for biobased chemicals, especially for more complex biobased chemicals. Second, detailed analysis of equipment costs, scaling factors, maximum scale, and total investment costs of the different industrial processing steps. Third, more insight into the inputs and especially the energy consumption of new industrial processes for the fermentation and recovery of novel biobased products. This also includes industrial pathways with multiple main products and more complex biorefinery concepts. In addition to improving the data quality and the availability of the biobased pathways more data are required regarding the fossil equivalent products and their production costs and GHG emission intensity. This study has quantified the GHG emission intensity and production costs of biobased ethanol, ethylene, 1,3-PDO, and succinic acid. To consider the overall sustainability of biobased fuels and chemicals, further aspects should be assessed, including land-use change GHG emissions, impact on water and biodiversity, and socio-economic aspects. The publication of uniform comparisons of the economic and GHG emission performance, or the wider sustainability performance, of different biobased production pathways can provide direction to reduce GHG emissions with biomass use or make an economically attractive business case.

Supporting information

File S1. Economic performance and GHG emission intensity of sugarcane- and eucalyptus-derived biofuels and biobased chemicals in Brazil.

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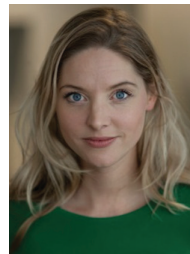
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