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LCA FOR ENERGY SYSTEMS AND FOOD PRODUCTS

Life cycle assessment of an integrated xylitol biorefinery with value-added co-products

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Abstract

Purpose This manuscript comprises a detailed life cycle assessment of an integrated xylitol biorefinery with value-added co-products. The biorefinery utilizes wheat straw as lignocellulosic feedstock and employs bio-based processes to produce xylitol as the main product and succinic acid as a co-product. The biorefinery was conceptually designed in an optimization-based framework and assessed through a techno-economic analysis published in the authors' prior publications.

Methods The goal is to determine the environmental impacts of the xylitol biorefinery and to compare the effects of bio-based production in the biorefinery to the current chemical production processes of xylitol. The scope is set as cradle-to-gate to allow a direct comparison of the chemical processes. The presented life cycle assessment was performed according to the standardized ISO procedure.

Results The reference unit is related to the feedstock as multiple products are produced, and an economic allocation is chosen. The life cycle inventory is based on secondary data from process simulations stemming from earlier published work. The impact assessment is performed with the ReCiPe 2016 Midpoint H V1.05 method and the IMPACT2002 + method since the available data of the life cycle assessment for the chemical processes was obtained with the latter. The characterization of the impacts shows high impacts for the terrestrial, marine, and human carcinogenic toxicity impact categories and a comparatively low impact on global warming.

Conclusions The results are interpreted and assessed with an additional sensitivity analysis. Furthermore, the results are compared with the two chemical production processes. The comparison shows lower impacts of the xylitol biorefinery compared to the standard chemical production process but slightly higher impacts compared to the proprietary production process of DuPont, which employs a high level of process integration. These results are further discussed and contextualized.

Keywords Biorefinery · Process design · Life cycle assessment · Cradle-to-gate · Xylitol · Succinic acid · Sensitivity analysis

1 Introduction

One of the overarching political, industrial, and also societal aims of our generation is the sustainable transition. On a global level, the United Nations have agreed upon 17 sustainable development goals, reaching from the eradication of hunger and poverty, the global access to clean freshwater and education up to the sustainable production of energy and sustainable production patterns, as well as general climate action (United Nations 2015). More sustainable production patterns, including concepts such as circular economy and resource recovery, and bio-based processes, are considered vital elements in the sustainable transition (De Jong et al. 2020; Lieder and Rashid 2016; Singh and Ordoñez 2016 United Nations 2015).

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In comparison to existing chemical production processes with fossil resources as feedstock, bio-based processes are deemed to be more sustainable due to milder process conditions, lower use of potentially harmful chemicals, and lower CO_2 emissions (Gavrilescu and Chisti 2005; Lokko et al. 2018; Woodley 2020). A particular concept in this context is biorefineries, analog to a fossil refinery, producing multiple products such as chemicals, fuels, and energy based on renewable feedstocks (Cherubini 2010). The palette of feedstocks is vast; hence, biorefineries are commonly classified into generations, depending on the feedstock: while first-generation biorefineries utilize food crops containing starch or glucose, second-generation biorefineries utilize crop residues or non-food crops (Cherubini 2010; Cherubini et al. 2009; Straathof et al. 2019).

Regarding the sustainability aspects of such biorefineries, while their sustainability potential, in general, seems promising, there are several aspects to consider. Despite around a thousand of them being implemented worldwide, first-generation biorefineries significantly impact the food-vs-fuel nexus (Naik et al. 2010; Rosegrant et al. 2006). Hence, considering an increased implementation of such biorefineries for the large-scale production of biofuels does stand diametrically to the SDGs, e.g., to the goal of eradicating hunger (Rosegrant et al. 2006). In addition, their sustainability potential in terms of, e.g., greenhouse gas emissions is less prevailing than for higher-generation biorefineries (Naik et al. 2010).

This particular issue shows that sustainability and the transition towards it are multi-faceted challenges and that changes in a specific part of a system can lead to subsequent effects in other parts of the system. Despite this, most sustainability analyses, mainly referred to as life cycle assessments (LCAs), are commonly focused on specific impacts and have unclear allocation methods and system boundaries, and do not analyze the entire system (Cherubini and Jungmeier 2010; Cherubini and Ulgiati 2010; Liu et al. 2021).

A potential example of a chemical production process that a biotechnological process can possibly replace is the production of xylitol. According to an evaluation of the US Department of Energy, xylitol is one of the top 12 chemicals to be produced in a biorefinery (Werpy and Petersen 2004). It can be used either as a building block for plastics or as a product for nutritional purposes, e.g., as a sugar substitute with several beneficial health properties (Da Silva and Chandel 2012; Hernández-Pérez et al. 2019). The current chemical production process utilizes lignocellulosic biomass as feedstock and is based on a chemical conversion process that requires high purities, making the upstream process quite complex and the product itself rather expensive (Delgado Arcaño et al. 2020; IMARC 2021).

Alternatively, xylitol could be produced in a biotechnological process, using lignocellulosic biomass as feedstock, but employing a fermentation unit instead of chemical conversion, tolerating higher levels of impurities with suitable microorganisms. Up to this date, most experimental studies proved this process to be feasible at laboratory scales. In contrast, conceptual studies regarding a technologically and economically viable process at a commercial scale are scarce. Vollmer et al. (2022a, b, c) have developed a conceptual process design for a xylitol biorefinery process with value-added co-products based on a synergistic optimization-based framework, including as much detailed knowledge about the process as possible/available (Vollmer et al. 2022a, c). The biorefinery concept uses wheat straw as lignocellulosic feedstock and employs bio-based processes to produce xylitol as the main product and succinic acid as a co-product. The lignin residues are burned to generate heat and electricity both of which are used internally in the process. While the process is technologically viable, its economic feasibility depends heavily on the present uncertainties regarding capital expenditures, operational expenses, and market conditions, particularly product prices.

To the best of our knowledge, previous LCA studies of xylitol production from bio-based sources and through fermentative processes have focused primarily on using corncob as a substrate. Both (Dasgupta et al. 2021) and the white report by DuPont (DuPont 2012) detail the impacts of the microbial fermentation of xylitol. The latter report also focuses on presenting the environmental impact of the currently used chemical route production process of xylitol.

Therefore, for a sound and proper assessment regarding the sustainability potential of the novel proposed xylitol biorefinery using lignocellulosic feedstock, an LCA will be performed in the scope of this paper. Based on the obtained LCA results, a comparison with the LCA results of the chemical process will allow for a detailed comparison of the different processes and facilitate conclusions regarding the potential of implementing biotechnological processes as an alternative to chemical ones in this specific case, but also in general. This facilitates a decision on whether implementing such a biorefinery process as an alternative to a chemical equivalent can be considered a positive development from an environmental sustainability perspective.

The remainder of this paper is structured as follows: in "Sect. 2," first, a detailed overview of the current chemical production process of xylitol is given. "Sect. 3" provides an overview of the goal and scope of the study, as well as a detailed explanation of the mentioned xylitol biorefinery based on a biotechnological process. In "Sect. 4," the detailed results of all four steps of the LCA for the xylitol biorefinery are presented. Subsequently, the results are compared to those of the chemical process. Lastly, in "Sect. 5," conclusions for the xylitol biorefinery in specific and also general conclusions are drawn.

2 Background

2.1 Current xylitol production

As of today, xylitol is exclusively produced in a chemical conversion process. Delgado Arcaño et al. (2020) describe it as follows: the single reaction step is the catalytic hydrogenation of xylose into xylitol over a Raney nickel catalyst at a temperature of around $T = 400\text{K}$ and $p = 50\text{bar}$ hydrogen pressure (Albuquerque et al. 2014; Delgado Arcaño et al. 2020). The yield of this conversion is around 98%, allowing for a simple downstream process, including a filtration, ion exchange, and crystallization unit. The xylose monomers are obtained from lignocellulosic biomass in a pretreatment unit; the hemicellulosic fraction of the lignocellulosic biomass is fractionated and depolymerized (Vollmer et al. 2022b). Due to the high sensitivity of the catalyst and to prevent an accelerated degradation after the pretreatment step, an intensive purification of the process stream is necessary to remove undesired by-products. The necessary purification before the reaction and the high temperature and pressure requirements have a substantial economic and significant sustainability impact on the entire production process and the final product price (Delgado Arcaño et al. 2020). Commonly, the used lignocellulosic biomass is either corncob or derives from birch trees, depending on the producer: several Chinese companies employ corncob as their feedstock, while DuPont Danisco utilizes the side stream of a paper mill, which utilizes the named birch trees (Hernández-Pérez et al. 2019).

A potential alternative to the chemical production process of xylitol is the production via a biotechnological process route. Hernández-Perez et al. (2019) describe it as follows: the feedstock for the biotechnological process route is also lignocellulosic biomass and involves the same biomass pretreatment unit to obtain xylose monomers as hydrolysate. As opposed to the chemical production route, an extensive purification of the obtained monomers is not required due to the higher resilience of microorganisms towards impurities compared to the catalyst. However, higher concentrations of certain inhibitory compounds, which are formed in the pretreatment, can negatively influence the performance of the microorganisms. Hence, either detoxification of the hydrolysate or an adaption of the cell factory through engineering strategies might be necessary. The following biotechnological conversion reaction through microorganisms, also called fermentation, occurs under much milder conditions—i.e., lower pressures and temperatures—than the chemical process. Commonly used microorganisms are different yeasts, e.g., *Candida*, *Debaryomyces*, or *Kluyveromyces* species, or engineered cell factories, e.g., engineered *Saccharomyces cerevisiae*. The yield of xylitol from xylose reaches from 45% in wild-type microorganisms to up to 90% in engineered microorganisms. In the downstream processing, after removing the cell biomass, the water content is commonly reduced before the purification of the xylitol. For the final purification step, crystallization units are a viable option (Hernández-Pérez et al. 2019). As mentioned, the biotechnological production of xylitol is not yet commercialized. Existing studies primarily focus on investigating the pretreatment, microorganisms, and initial studies regarding the entire process, pointing out a need for more conceptual investigations (Albuquerque et al. 2014; Dasgupta et al. 2017; Hernández-Pérez et al. 2019; Rao et al. 2016).

3 Materials and methods

3.1 Definitions of goal and scope

The study was performed based on the ISO 14040 guidelines (Standard 2006—ISO) and described by Hauschild et al. (2017), and accordingly, the first step is the definition of goal and scope of the study. In this work, for the xylitol biorefinery, the goal of the LCA is to evaluate the environmental sustainability impacts to identify the potential environmental improvements of the xylitol production via a biotechnological process route over the existing chemical one. The function of the system is the annual production of $m = 12186\text{t}$ of food-grade xylitol. Since succinic acid is a value-added co-product, its production is also included in the scope of the LCA. For simplicity regarding the calculations and to include all co-products, the reference flow is thus defined as the feedstock and accounted for as $m = 1\text{t}$. As the xylitol biorefinery processes $m = 150,000\text{t}$ of wheat straw annually, all other streams are normalized with that number. The scope is set as "cradle-to-gate" to enable a precise comparison to the chemical process and exclude other auxiliary factors.

3.1.1 General process description: xylitol biorefinery

Based on this general evaluation, in a previous publication, the authors conducted a study on the conceptual process design of a xylitol biorefinery—the biotechnological production of xylitol in an integrated biorefinery setup with value-added co-products. Vollmer et al. (2022a, b, c) describe the conceptual process design: xylitol is the primary product and the hemicellulosic fraction of the used lignocellulosic biomass—in this case, wheat straw—is used for its production. In order to utilize the feedstock to the maximum extent possible, the cellulosic and lignin fractions are also used for the production of respectively succinic acid and combustion for the generation of steam and electricity. The aims of this process integration step are twofold: firstly, it aims at improving the economic performance of the plant by reducing the net amount of steam and electricity needed, and secondly, to improve the sustainability potential.

After a biomass pretreatment unit, the xylitol process train is composed similarly; the pretreatment follows an evaporation unit that serves the upconcentration of the hydrolysate and the removal of volatile inhibitory compounds. After that, the fermentation unit follows. In the downstream process, after the removal of the cells, firstly, an evaporation unit reduces the amount of water in the process stream and is followed by two crystallization units to purify the product. Also, after the biomass pretreatment, the remaining solid fraction is transferred towards an enzymatic hydrolysis unit, which fractionates the cellulosic fraction and depolymerizes it. The following process steps are the same as for the xylitol process train. The only difference is that the produced product is succinic acid, and the operation mode of the second crystallization is another cooling crystallization instead of an antisolvent crystallization. After the enzymatic hydrolysis, the lignin is transferred to combustion with an included steam and power generation unit. Furthermore, the xylitol biorefinery comprises a wastewater treatment unit (Vollmer et al. 2022c). The entire conceptual process flowsheet, partly excluding the auxiliary unit operations, is displayed in Fig. 1.

The entire flowsheet has been designed in a synergistic optimization-based framework for the conceptual process design of biorefineries and is thus composed of different mathematical models (Vollmer et al. 2022a). The framework and the models for the xylitol biorefinery are made available through a GitHub repository, together with the calculation files for the LCA (Vollmer 2022).

Noteworthy from a sustainability perspective besides the implemented process integration is that the microorganisms in the succinic acid fermentation take up CO_2 based on the process stoichiometry. Technically, this is achieved by using CO_2 from potentially fossil sources and sparging it in the fermentation reactor. Hence, the process has a net negative CO_2 balance. As mentioned in “Sect. 1,” while an extensive techno-economic analysis regarding the economic viability of the biorefinery has been performed, the sustainability potential of this biorefinery in specific, or such biorefinery concepts in general, has yet to be investigated comprehensively with several impact factors.

3.2 Life cycle inventory analysis

Once the goal, scope, system boundaries, and functional unit have been determined, the next step is to establish the life cycle inventory (LCI). LCI analysis serves to quantify all input and output flows to and from the analyzed system. Through the quantification, a comprehensive inventory of the system is obtained. The flows comprise both mass flows in all states and energy flows. Also, the allocation is performed in this step: if several products are produced, a decision on how the impacts are weighed among the products has to be taken. Typical examples are mass-based or economy-based allocation.

Firstly, for the LCI, a flowsheet simulation with the existing models is performed to determine all flows into and out of the system. The principal input is the wheat straw as

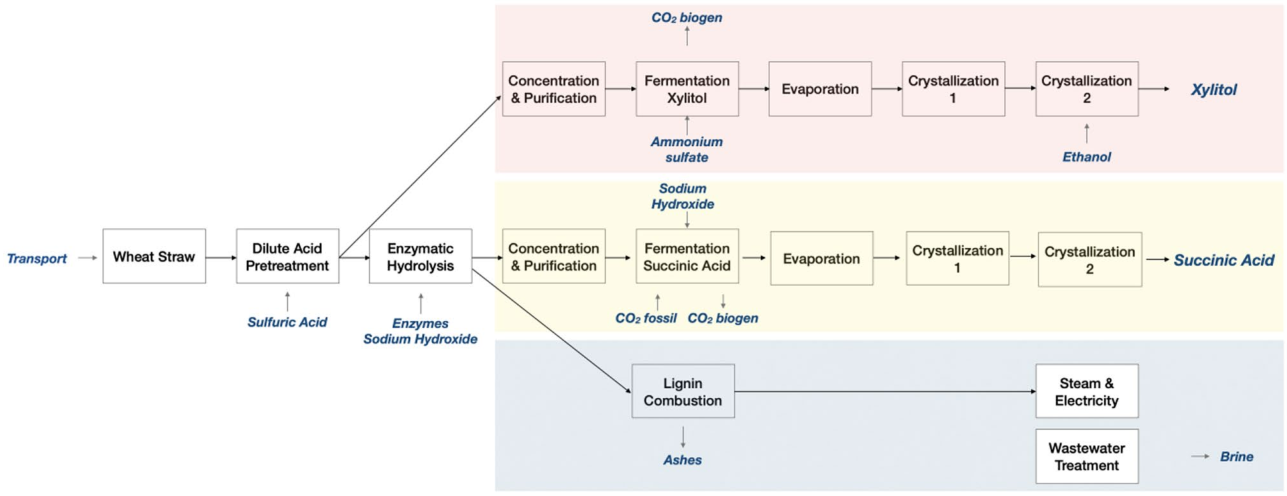


Fig. 1 Conceptual process flowsheet of the xylitol biorefinery with input and output flows

feedstock. For the pretreatment unit, a flow of sulfuric acid is accounted. For the enzymatic hydrolysis, a flow of sodium hydroxide and the flow of the enzymes are accounted. Subsequently, both fermentations account for additional sodium hydroxide for the neutralization and titration and ammonium sulfate as the nitrogen source for the fermentation. In addition, for the succinic acid fermentation, a stream of fossil CO_2 is considered. Furthermore, ethanol as the antisolvent in the second crystallization step is included for the downstream process of the xylitol process train. Moreover, the overall process requires a net stream of process water, in addition to the internal recovery, as well as a net stream of medium-pressure steam in addition to the internally generated steam and a certain amount of electricity in addition to the internally generated electricity. Of note is that the auxiliary combined heat and power unit (CHP) for the combustion of lignin has not been modeled separately; hence, there are no direct emissions linked to this step. Indeed, the corresponding emissions for the utility consumptions are accounted for from the ReCiPe database. Lastly, make-up streams for the cooling and chilling water are included in addition to the internal recovery.

For the transport of the wheat straw to the factory, an average distance of 100km is assumed for a fictional location of the biorefinery in Denmark. The flows out of the biorefinery that are accounted for are the products xylitol and succinic acid. Moreover, waste brine as a residual outflow from the wastewater treatment and ashes from the combustion process are assumed, together with biogenic CO_2 as a by-product from the fermentations.

Table 1 Annual inputs and outputs to the system

Inputs from technosphere			Outputs to technosphere		
Materials			Products		
Wheat straw (dry)	150,000	t	Xylitol	12,186	t
Sulfuric acid	17,756	t	Succinic acid	19,220	t
Enzymes	2591	t			
Ammonium sulfate	13	t			
Sodium hydroxide	827	t			
Process water	21,419	t			
Ethanol	2592	t			
CO_2 (fossil)	1551	t			
Transport			Waste		
To plant	15,000,000	t • km	Waste brine	59,576	t
			Ashes	911	t
Energy			Emissions		
Steam (MP)	1,611,300	t	CO_2 (biogen)	523	t
Electricity	78,732,000	MJ			
Cooling water	2,407,300	t			
Chilling water	6.77	t			

The flows are retrieved from a flowsheet simulation with the existing models and hence are secondary data and do not stem from a biorefinery directly, as this study is conceptual and no commercial process exists yet. All flows are listed in Table 1.

According to Cherubini and Jungmeier (2010), many LCA studies partition the results using an economic basis where the basic idea is that the actual cause for establishing a multifunctional process is followed, and it is the economic profitability. Furthermore, as highlighted in Pelletier et al. (2015) and Ardente and Cellura (2012), an argument is that economic allocation is proper when co-products have intrinsic qualities that physical parameters cannot adequately reflect.

Thus, in this work, the allocation of the products for the LCA is chosen to be economy-based. All flows are normalized with the reference stream. Figure 1 illustrates all flows in and out of the system according to their unit operations.

4 Results

4.1 Life cycle impact assessment

Through this third step, life cycle impact assessment (LCIA), all elements in the inventory are classified and characterized over all impact categories based on their contribution to respective environmental effects.

Table 2 Impact categories of the ReCiPe 2016 Midpoint H V1.05 database

Impact category	Unit	Category abbreviation
Global warming	kgCO$_2$eq	GW
Ozone depletion	kgCFC – 11eq	OD
Ionizing radiation	kBqCo – 60eq	IR
Ozone formation, human health	kgNO$_x$eq	OH
Fine particular matter formation	kgPM2.5eq	FP
Ozone formation, terrestrial ecosystems	kgNO$_x$eq	OT
Terrestrial acidification	kgSO$_2$eq	TA
Freshwater eutrophication	kgPeq	FT
Marine eutrophication	kgNeq	MT
Terrestrial ecotoxicity	kg1, 4 – DCB	TE
Freshwater ecotoxicity	kg1, 4 – DCB	FE
Marine ecotoxicity	kg1, 4 – DCB	ME
Human carcinogenic toxicity	kg1, 4 – DCB	HC
Human non-carcinogenic toxicity	kg1, 4 – DCB	HN
Land use	m^{2}acropeq	LU
Mineral resource scarcity	kgCueq	MR
Fossil resource scarcity	kgoileq	FR
Water consumption	m^3	WC

Table 3 Processes from the Ecoinvent 3 database with their according names

Process number	Units	Ecoinvent 3.6 database processes
1	kg	Wheat Straw at Farm/DK
2	kg	Sulfuric Acid (RER), production of sulfuric acid cut-off (S)
3	kg	Enzyme, Cellulase, Novozymes Celluclast/kg/RER
4	kg	Ammonium Sulfate (RER), ammonium sulfate production cut-off (S)
5	kg	Sodium hydroxide, without water, in 50% solution state {RER}| chlor-alkali electrolysis, diaphragm cell | Cut-off, S
6	kg	Water, deionised {Europe without Switzerland}| market for water, deionised | Cut-off, S
7	kg	Ethanol, without water, in 99.7% solution state, from ethylene {RER}| ethylene hydration | Cut-off, S
8	kg	Carbon dioxide, liquid {RER}| production | Cut-off, S
9	kg	Sodium chloride, brine solution {RER}| production | Cut-off, S
10	kg	Ash, from combustion of bagasse from sugarcane {GLO}| market for ash, from combustion of bagasse from sugarcane | Cut-off, S
11	t • km	Transport, freight, lorry > 32 metric ton, EURO4 {RER}| transport, freight, lorry > 32 metric ton, EURO4 | Cut-off, S
12	kg	Steam, in chemical industry {RER}| production | Cut-off, S
13	MJ	Electricity, high voltage {DK}| electricity production, wind, > 3 MW turbine, onshore | Cut-off, S
14	kg	Tap water {RER}| market group for | Cut-off, S
15	kg	Tap water {RER}| market group for | Cut-off, S
16	kg	CO2 fossil
17	kg	CO2 biogen

In this study, the results of the LCI were modeled using ReCiPe 2016 Midpoint H V1.05 method (Huijbregts et al. 2017). The ReCiPe method considers 18 impact categories. They are listed in Table 2.

All inventory items for the processes in Table 3 are retrieved from the Ecoinvent 3.6 database, except process numbers 3, 16, and 17. The characterized results for the enzymes stem from a proprietary study of Novozymes (Nielsen et al. 2007). The fossil and biogenic CO_2 values for the GW impact are set to a standard definition ($CO_{2,\text{fossil}} = -1, CO_{2,\text{biogenic}} = 0$), as CO_2 is the reference component for the global warming impact category in the ReCiPe methodology. The respective processes for the flows are listed in Table 3.

The contribution of each process to each impact category is calculated and then scaled to the reference flow. The results of calculating the impacts for each process number with the characterization factors are listed in Table 4. The results of the LCIA for the three highest impacts in each category are displayed in Fig. 2, while the rest is ignored due to marginal relative impacts in the respective category.

It becomes apparent, that only six out of seventeen processes have a significant relative impact in these categories, namely, the wheat straw, the transport, the waste brine, the steam, the electricity, and the cooling water.

The normalization of the LCIA results is done by the ReCiPe Midpoint World (2010) H (V1.05), corresponding to the sustainability impact of one global citizen. The results for the categories with a normalized impact bigger than $1 \cdot 10^{-1}$ for the respective categories are displayed in Fig. 3. The normalization values are displayed as fractions to the normalization value.

It becomes visible that the most significant impacts when normalized occur in the categories freshwater ecotoxicity, marine ecotoxicity, human carcinogenic toxicity, and water consumption. Furthermore, according to Guinée et al. (2004), economic allocation is the advised baseline method. Thus, the economic allocation with a market price of 4.81$/kg and 3.20$/kg for xylitol and succinic acid, the economic allocation has distributed 48.8% of the impact on the xylitol production and 51.2% on the succinic acid production.

Note that the calculation of all four steps is performed in MATLAB; all simulation files are provided through a GitHub repository for the interested reader (Vollmer 2022).

4.2 Sensitivity analysis on the LCIA results

In this work, a complementary sensitivity analysis is performed to obtain a more detailed picture for the interpretation of results (Hauschild et al. 2017).

For the sensitivity analysis of the characterization results of the LCIA, all inputs, as indicated in Table 1, are considered randomly distributed by ±15% around their nominal value. With the flowsheet model, $N = 1000$ simulations are performed to obtain the characterization results with the according characterization factors. Using the easyGSA

Table 4 Results for the characterization in the LCIA

	GW kgCO$_2$eq	OD kgCFC − 11eq	IR kBqCo − 60eq	OH kgNO$_x$eq	FP kgPM2.5eq	OT kgNO$_x$eq	TA kgSO$_2$eq	FT kgPeq	MT kgNeq
1	2.84e−1	6.73e−6	6.21e−4	5.32e−4	5.39e−4	5.36e−4	3.92e−3	1.05e−4	2.10e−3
2	1.98e−2	1.21e−8	1.01e−3	1.30e−4	2.21e−4	1.33e−4	7.12e−4	2.33e−5	9.65e−7
3	7.06e−2	0.00	0.00	1.26e−5	7.65e−5	2.03e−5	2.64e−4	5.34e−6	0.00
4	1.03e−4	3.19e−11	9.01e−6	1.84e−7	2.75e−7	1.94e−7	9.67e−7	3.99e−8	1.03e−7
5	7.24e−3	7.70e−9	7.91e−4	1.90e−5	1.56e−5	1.92e−5	2.62e−5	3.55e−6	3.62e−7
6	6.49e−5	6.24e−11	5.90e−6	1.35e−7	1.67e−7	1.38e−7	4.20e−7	2.39e−8	2.76e−9
7	1.94e−2	1.77e−7	5.80e−4	7.75e−5	5.58e−5	8.09e−5	1.99e−4	6.11e−6	3.81e−5
8	7.62e−3	1.53e−9	8.97e−4	7.15e−6	4.89e−6	7.30e−6	1.21e−5	2.33e−6	4.88e−7
9	9.95e−2	3.92e−8	1.15e−2	2.60e−4	2.14e−4	2.65e−4	4.22e−4	7.23e−5	3.97e−6
10	4.07e−6	1.84e−12	7.92e−8	2.21e−8	5.83e−9	2.26e−8	1.35e−8	3.46e−10	3.05e−11
11	4.07e−6	1.84e−12	7.92e−8	2.21e−8	5.83e−9	2.26e−8	1.35e−8	3.46e−10	3.05e−11
12	8.66	6.32e−6	2.09e−1	1.73e−2	9.05e−3	1.83e−2	1.76e−2	5.90e−4	5.43e−5
13	3.08	7.49e−7	7.32e−2	3.72e−3	2.36e−3	3.82e−3	6.97e−3	2.98e−4	2.04e−5
14	2.89	1.34e−6	1.40e−1	1.02e−2	6.34e−3	1.05e−2	1.25e−2	2.93e−3	2.08e−4
15	5.47e−3	2.37e−9	1.73e−3	1.29e−5	9.16e−6	1.33e−5	2.03e−5	3.97e−6	3.78e−7
16	1.54e−8	6.67e−15	4.86e−9	3.64e−11	2.58e−11	3.74e−11	5.72e−11	1.12e−11	1.06e−12
17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	2.53E+01	0.00E+00	2.68E+00	8.00E−02	4.00E−02	8.00E−02	1.00E−02	0.00E+00	6.67E+00

	TE kg1, 4 − DCB	FE kg1, 4 − DCB	ME kg1, 4 − DCB	HC kg1, 4 − DCB	HN kg1, 4 − DCB	LU m^{2}acropeq	MR kgCueq	FR kgoileq	WC m^3
1	2.26e−1	1.75e−2	3.61e−3	1.15e−4	2.81	9.17e−1	1.21e−4	2.82e−2	4.47e−3
2	4.81e−1	3.92e−3	5.75e−3	1.91e−3	1.99e−1	9.51e−4	4.71e−4	1.70e−2	2.50e−3
3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.98e−2	3.60e−4
4	5.46e−4	1.85e−5	2.15e−5	1.77e−5	2.47e−4	3.52e−6	1.27e−6	3.88e−5	3.08e−6
5	1.38e−2	4.01e−4	5.22e−4	5.96e−4	8.43e−3	1.66e−4	2.30e−5	1.80e−3	1.90e−4
6	2.18e−4	4.04e−6	5.32e−6	9.13e−6	8.27e−5	1.44e−6	4.34e−7	1.83e−5	1.50e−4
7	4.67e−2	1.08e−3	9.30e−4	1.16e−3	2.98e−2	2.69e−2	8.71e−5	4.04e−3	2.74e−3
8	4.39e−2	4.08e−4	5.17e−4	4.84e−4	6.71e−3	1.28e−4	2.71e−5	1.34e−3	5.55e−5
9	4.79e−1	2.79e−2	3.54e−2	2.94e−2	3.98e−1	6.63e−3	2.05e−3	2.44e−2	−1.11
10	7.64e−5	8.19e−8	1.50e−7	2.41e−7	2.92e−6	2.25e−7	7.66e−9	1.41e−6	e−4
11	7.64e−5	8.19e−8	1.50e−7	2.41e−7	2.92e−6	2.25e−7	7.66e−9	1.41e−6	7.64e−9
12	2.18e2	1.43e−1	3.06e−1	4.63e−1	5.69	6.85e−1	1.33e−2	3.21	1.64e−2
13	4.41	1.42e−2	2.46e−2	4.89e−2	5.28e−1	2.66e−2	7.20e−4	1.03	3.22e−3
14	2.34e1	6.50	7.87	2.48	2.38e1	1.73e−1	1.23e−1	7.08e−1	3.78e−2
15	1.25e−2	2.80e−4	3.85e−4	4.30e−3	6.63e−3	1.41e−4	6.34e−5	1.45e−3	1.61e−2
16	3.51e−8	7.88e−10	1.08e−9	1.21e−8	1.86e−8	3.97e−10	1.78e−10	4.07e−9	4.54e−8
17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	8.23E+01	2.57E+00	4.00E−01	7.62E+00	1.61E+01	2.53E+01	0.00E+00	2.68E+00	8.00E−02

toolbox, applying a variance-based sensitivity analysis, the first-order and the total sensitivity indices are calculated. A detailed description of the sensitivity analysis methodology and the presented toolbox can be found in Al et al. (2019). The results for the total sensitivity index are illustrated in Fig. 4.

It is visible that electricity, which influences the results of the LCIA the most, shows only low sensitivity indices. The amount of feedstock, i.e., the wheat straw, influences the most important impact categories, freshwater and marine ecotoxicity as well as the human carcinogenic potential. The two former result from the use of pesticides in agriculture while the latter results from particles and VOCs from diesel burning. These are all processes that have a high impact and consequently sensitive. The transportation distance also to a large extent has a significant effect on all these three impact

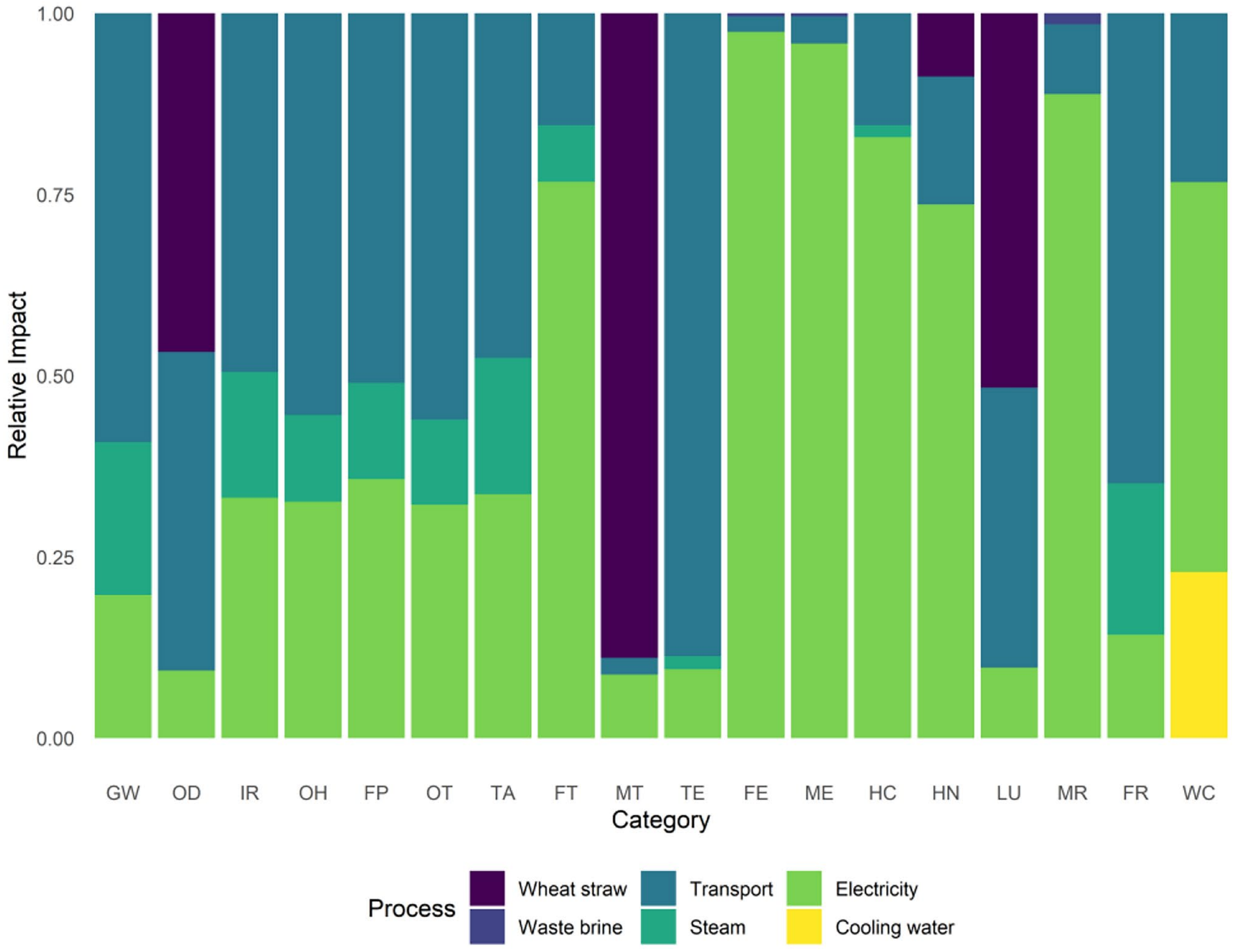


Fig. 2 LCIA results of the characterization given in percentages for each category

categories, partly due to emissions from tire wear as well as the particles and VOC from diesel burning. The effect on the marine ecotoxicity of the higher use of cooling water can also be attributed to the use of electricity in the process.

4.3 Interpretation of results

Given the results displayed in Fig. 3, it becomes evident that the impact of the xylitol biorefinery on global warming is minimal. This is in agreement with most studies regarding biorefineries and also one of the main assumptions regarding bio-based processes in general, which is why they are promoted as more sustainable in the first place. However, while most impacts are relatively low, the impacts on freshwater toxicity, marine ecotoxicity, and human carcinogenic potential are substantially higher. This is an often seen (Bello et al. 2018; Hauschild et al. 2017).

As mentioned in "Sect. 4.2" and Fig. 3, the most significant impacts are freshwater ecotoxicity, marine ecotoxicity, human carcinogenic toxicity, and water consumption.

Figure 2 shows that only a few processes dominate the potential environmental impact categories (wheat straw, transport, waste brine, steam, the electricity, cooling water).

There are several aspects to consider when using wheat straw as a raw material; as any other lignocellulosic feedstock claimed as sustainable, it carries some environmental consequences. The cultivation of wheat straw (important consideration since this is a cradle-to-gate study) leads to the use of fertilizers, herbicides, and pesticides (and large amounts of water), which is detrimental to freshwater and marine ecotoxicity. Besides the use of these compounds, the rain and runoff from agricultural activities can and do carry these hazardous compounds to bodies of water, potentially harming freshwater and marine ecosystems (freshwater and marine ecotoxicity). Furthermore, wheat straw collection (harvest) and

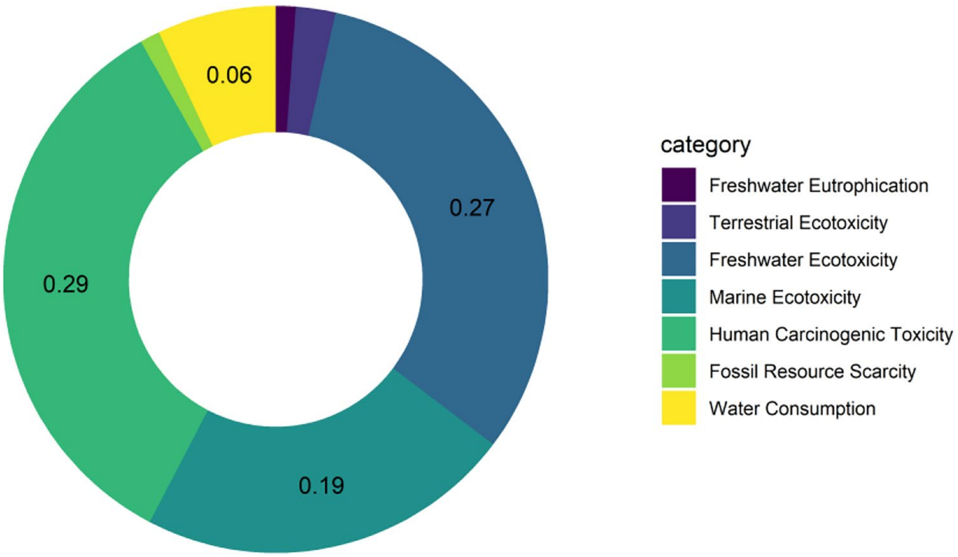


Fig. 3 Results of the LCIA with applied normalization

transport involve heavy transport trucks and machinery that consume considerable amounts of fuel leading to emissions of particulates and VOCs. Furthermore, of note is that during the breakdown process of wheat straw, there are also several toxic by-products that, if not collected and managed appropriately, can have the same destination through wastewater streams.

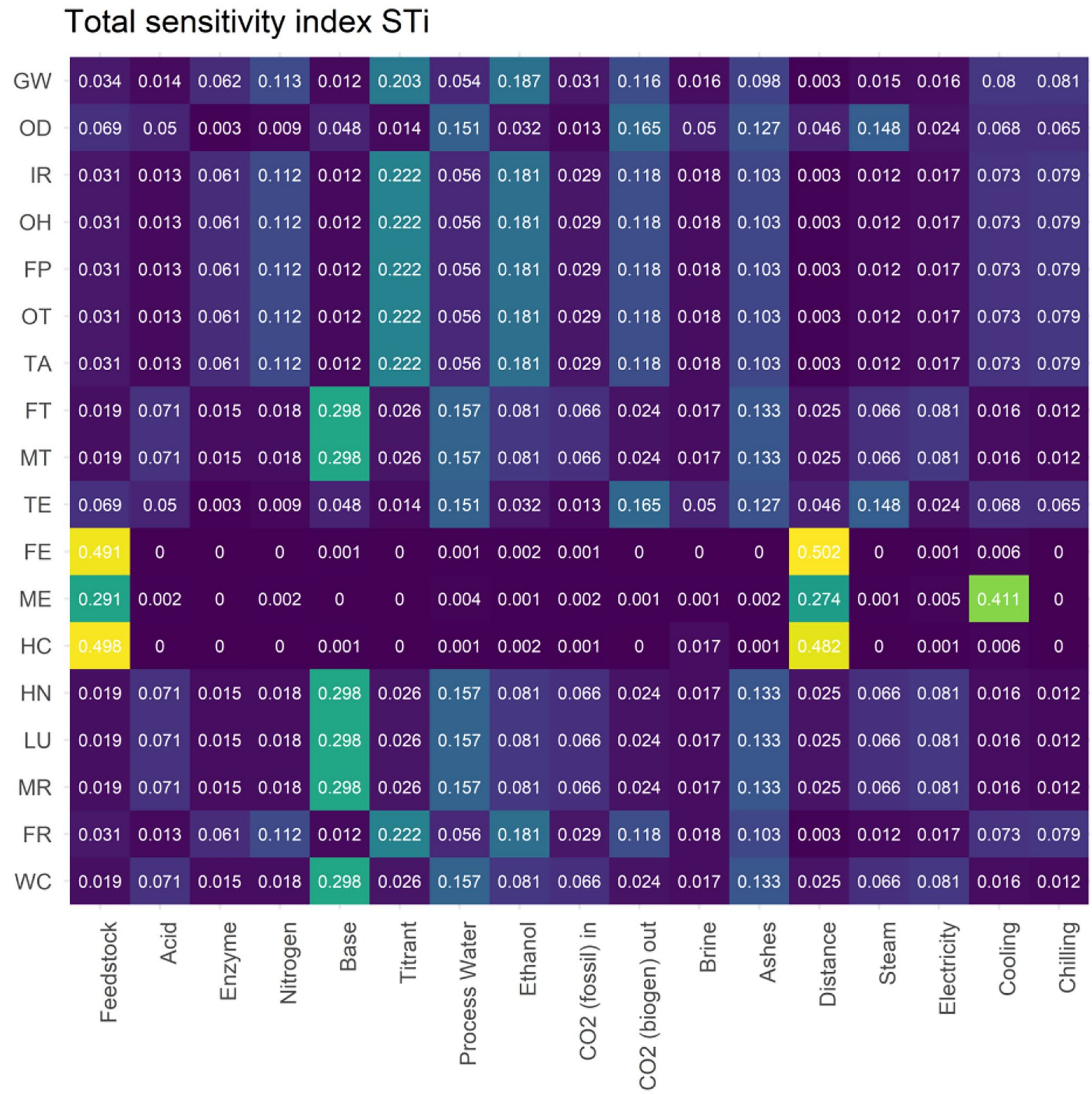
Analyzing those three impact categories in detail in Fig. 2, it is visible that more than 80% of the impact is associated with electricity. Given that the electricity is chosen to be generated by wind turbines, which are supposedly more sustainable and seen as a crucial element as part of national and global renewable energies, this seems initially contradictory. Of note is that wind turbines were chosen as the source of electricity generation in Denmark since offshore and onshore wind turbines have produced over 46% of Denmark's total electricity consumption in 2020 ("A record year: Wind and solar supplied more than half of Denmark's electricity in 2020," n.d.). Therefore, we believe it to be a realistic assumption that this biorefinery would run only, or primarily, on wind energy as a source for consumed electricity. Assessing the process of creating electric energy through wind turbines in the Ecoinvent 3 database shows that the major sustainability impact derives from using copper in the wind turbine generators. Although copper itself is a micronutrient for many species, the mining process of copper involves significant amounts of toxic chemicals, which, if not discarded correctly, can damage aquatic organisms (Fuentes et al. 2021; Nor 1987; Olivares and Uauy 1996). This issue is known and is a problem for the environment (Castilla and Nealler 1978; Covre et al. 2022; Lyu et al. 2018).

In order to illustrate these results, an example shall be given: taking into account the total characterized impact and the economic allocation, the production of 1kg of xylitol equals 12.3kg of CO_2 emissions, which is approximately half the emissions of the production of 1kg of beef, which equals 20–40 kg of CO_2 emissions, and around four times the emission of the production of 1kg of chocolate bars, which equals 3.5kg of CO_2 emissions (DuPont 2012).

4.4 Comparison to the current production process

Ultimately, to compare the biorefinery process with the existing chemical process, an LCA of Danisco DuPont regarding their process based on birch trees is taken from a whitepaper (DuPont 2012). In the white paper, both process setups are described and compared to the other commercial processes that utilize corncob instead of the side stream of a paper mill. This is a realization of process integration performed for the process of DuPont, improving the sustainability metrics (DuPont 2012). The used LCIA methodology in DuPont (2012) is IMPACT2002 + (Jolliet et al. 2003). Hence, the results of the LCIA for the xylitol biorefinery are also generated through this methodology in addition to the previously shown results by the ReCiPe methodology. The summed impact factors for each category for the entire process for DuPont's process, the corncob-based process, and the xylitol biorefinery are reported in Table 5. The set reference flow for the study conducted by DuPont is $m = 1$t of xylitol, with the same purity requirements, accounting also for the material and energy flows and the emissions caused by its production as cradle-to-gate (DuPont 2012).

Firstly, it becomes apparent that the impacts of the xylitol biorefinery show similar magnitudes for all impact categories compared to both chemical processes. Secondly, for all impact categories, the impacts of the xylitol biorefinery are



Total sensitivity index STi

	Feedstock	Acid	Enzyme	Nitrogen	Base	Titrant	Process Water	Ethanol	CO2 (fossil) in	CO2 (biogen) out	Brine	Ashes	Distance	Steam	Electricity	Cooling	Chilling
GW	0.034	0.014	0.062	0.113	0.012	0.203	0.054	0.187	0.031	0.116	0.016	0.098	0.003	0.015	0.016	0.08	0.081
OD	0.069	0.05	0.003	0.009	0.048	0.014	0.151	0.032	0.013	0.165	0.05	0.127	0.046	0.148	0.024	0.068	0.065
IR	0.031	0.013	0.061	0.112	0.012	0.222	0.056	0.181	0.029	0.118	0.018	0.103	0.003	0.012	0.017	0.073	0.079
OH	0.031	0.013	0.061	0.112	0.012	0.222	0.056	0.181	0.029	0.118	0.018	0.103	0.003	0.012	0.017	0.073	0.079
FP	0.031	0.013	0.061	0.112	0.012	0.222	0.056	0.181	0.029	0.118	0.018	0.103	0.003	0.012	0.017	0.073	0.079
OT	0.031	0.013	0.061	0.112	0.012	0.222	0.056	0.181	0.029	0.118	0.018	0.103	0.003	0.012	0.017	0.073	0.079
TA	0.031	0.013	0.061	0.112	0.012	0.222	0.056	0.181	0.029	0.118	0.018	0.103	0.003	0.012	0.017	0.073	0.079
FT	0.019	0.071	0.015	0.018	0.298	0.026	0.157	0.081	0.066	0.024	0.017	0.133	0.025	0.066	0.081	0.016	0.012
MT	0.019	0.071	0.015	0.018	0.298	0.026	0.157	0.081	0.066	0.024	0.017	0.133	0.025	0.066	0.081	0.016	0.012
TE	0.069	0.05	0.003	0.009	0.048	0.014	0.151	0.032	0.013	0.165	0.05	0.127	0.046	0.148	0.024	0.068	0.065
FE	0.491	0	0	0	0.001	0	0.001	0.002	0.001	0	0	0	0.502	0	0.001	0.006	0
ME	0.291	0.002	0	0.002	0	0	0.004	0.001	0.002	0.001	0.001	0.002	0.274	0.001	0.005	0.411	0
HC	0.498	0	0	0	0.001	0	0.001	0.002	0.001	0	0.017	0.001	0.482	0	0.001	0.006	0
HN	0.019	0.071	0.015	0.018	0.298	0.026	0.157	0.081	0.066	0.024	0.017	0.133	0.025	0.066	0.081	0.016	0.012
LU	0.019	0.071	0.015	0.018	0.298	0.026	0.157	0.081	0.066	0.024	0.017	0.133	0.025	0.066	0.081	0.016	0.012
MR	0.019	0.071	0.015	0.018	0.298	0.026	0.157	0.081	0.066	0.024	0.017	0.133	0.025	0.066	0.081	0.016	0.012
FR	0.031	0.013	0.061	0.112	0.012	0.222	0.056	0.181	0.029	0.118	0.018	0.103	0.003	0.012	0.017	0.073	0.079
WC	0.019	0.071	0.015	0.018	0.298	0.026	0.157	0.081	0.066	0.024	0.017	0.133	0.025	0.066	0.081	0.016	0.012

Fig. 4 Heat map of the first-order and total sensitivity indices for all process numbers and all impact categories

higher than for the DuPont process, which again shows lower impacts in all categories than the corncob process. This can be linked to the fact that DuPont's process is integrated into a pulp and paper mill and can significantly decrease the sustainability impact through this. This integration is investigated specifically by assessing the impacts only for the xylitol process train and disregarding the impacts associated with the succinic acid for a fair comparison to the xylitol biorefinery. For the energy flows, it is assumed that the net flows are reduced as the process integration for steam and electricity still yields identical amounts regardless of the succinic acid production but are not used for the succinic acid production. The flows that are exclusively needed for the production of succinic acid are subtracted from the material flows. For the cooling water, process water, and waste brine, the flows are reduced by 50% as they are only calculated for the entire biorefinery and cannot be split up precisely (Table 6).

Although the metrics for the xylitol process train only improved the overall sustainability impact, the impacts of the DuPont process are still generally lower, but all in

Table 5 LCIA of the results for the impacts in all categories for the DuPont process, the corncob process, and the xylitol biorefinery

Impact category	Unit	DuPont process (DuPont 2012)	Corncob process (DuPont 2012)	Xylitol biorefinery
Aquatic acidification	kgSO$_2$eq	0.00873	0.334	0.0551
Aquatic ecotoxicity	kgTEGwater	599	60,600	2463
Aquatic eutrophication	kgPO$_4$Plimited	0.00119	0.0512	0.0023
Carcinogens	kgC$_2$H$_3$Cleq	0.04119	0.283	0.3075
Global warming	kgCO$_2$eq	3.59	38.6	14.548
Ionizing radiation	BqC − 14eq	51.1	477	108.6
Land occupation	M2Org.Arable	0.0487	9.1	1.8854
Mineral extraction	MJsurplus	0.0623	0.435	1.7066
Non-carcinogens	kgC$_2$H$_3$Cleq	0.0335	1.18	1.2547
Non-renewable energy	MJprimary	66.8	454	238.655
Ozone layer depletion	kgCFC − 11eq	0.000563	0.00417	2.24e−6
Respiratory inorganics	kgPM2.5eq	0.00152	0.0433	0.0134
Respiratory organics	kgC$_2$H$_4$eq	0.000991	0.00606	0.0084
Terrestrial acid/nutria	kgSO$_2$eq	0.034	1.06	0.2283
Terrestrial ecotoxicity	kgTEGsoil	150	2660	1760

comparable orders of magnitude. However, it has to be pointed out that the biotechnological process route for xylitol production, as investigated in this study, is still conceptual. In the scale-up and commercialization process of new plants, potentials for optimizing the process from an economic and environmental perspective are commonly leveraged (Bergerson et al. 2020; Piccinno et al. 2016).

In summary, this study poses certain limitations directly linked to the sole use of secondary data to build the LCI. The following limitations are noted:

(a) The use of secondary data is probably not fully representative of the process, where products and emissions can, for instance, be missing or misrepresented. The data must be updated based on technical/technological development.

(b) This data may not entirely represent the temporal and geographical boundaries. Updates based on the industry and market should also be taken into account.

(c) The compounding effect derived from it being a process at the early stage of design where all parameters have inbuilt uncertainty.

Table 6 LCIA of the results for the impacts in all categories for the DuPont process and the xylitol process train of the xylitol biorefinery

Impact category	Unit	DuPont process (DuPont 2012)	Xylitol process train	DuPont/xylitol
Aquatic acidification	kgSO$_2$eq	0.00873	0.0342	25.5%
Aquatic ecotoxicity	kgTEGwater	599	1391	43.1%
Aquatic eutrophication	kgPO$_4$Plimited	0.00119	0.0013	91.5%
Carcinogens	kgC$_2$H$_3$Cleq	0.04119	0.0774	53.2%
Global warming	kgCO$_2$eq	3.59	10.7783	33.3%
Ionizing radiation	BqC − 14eq	51.1	83.3113	61.3%
Land occupation	M2Org.Arable	0.0487	1.7175	2.84%
Mineral extraction	MJsurplus	0.0623	0.0838	74.3%
Non-carcinogens	kgC$_2$H$_3$Cleq	0.0335	0.5223	6.41%
Non-renewable energy	MJprimary	66.8	186.369	35.8%
Ozone layer depletion	kgCFC − 11eq	0.000563	1.94e−6	−290%
Respiratory inorganics	kgPM2.5eq	0.00152	0.0082	18.5%
Respiratory organics	kgC$_2$H$_4$eq	0.000991	0.0062	16.0%
Terrestrial acid/nutria	kgSO$_2$eq	0.034	0.1512	22.5%
Terrestrial ecotoxicity	kgTEGsoil	150	1491	10.0%

The data's fitness to purpose is paramount; therefore, the proposed process analysis will benefit from further investigation and validation ideally with primary data such as demonstration/production scale data. This is especially relevant during the final stages and the commercialization phase to optimize the flows and reduce the sustainability impact.

5 Conclusions

In the scope of this manuscript, a systematic LCA is performed for an integrated xylitol biorefinery with value-added co-products. The goal of the LCA is to evaluate the environmental impacts of xylitol production via a biotechnological process route in an integrated biorefinery setup with value-added co-products and compare the impacts to the existing chemical xylitol production process. The LCA is performed according to the four-step procedure as defined in ISO 14040. The xylitol biorefinery utilizes wheat straw as renewable feedstock. It involves a pretreatment unit and an enzymatic hydrolysis unit in the upstream process, two fermentation units for the biotechnological conversion of the feedstock to xylitol and succinic acid, respectively, and in each downstream process, an evaporation unit and two crystallization units for the purification of the products.

Additionally, auxiliary unit operations are considered, e.g., a combustion unit for lignin to generate steam and electricity as a process integration strategy and a wastewater treatment unit. The results of the LCA show that while the process generally shows low impacts, particularly regarding greenhouse gas emissions, other categories show higher impacts. These results are compared to two types of chemical production processes. While the xylitol biorefinery process has lower impacts than the standard chemical conversion process, it has higher impacts than a process integrated into a pulp and paper mill operated by DuPont.

This leads to the conclusion that the biotechnological production process per se is not more sustainable than the chemical one. When comparing it to the existing chemical process, the sustainability potential becomes apparent, while this fact is not directly visible compared to the DuPont process. Compared to the classic chemical one, the DuPont process employs the same reaction system but heavily employs process integration measures by being located adjoint to a pulp and paper mill. The white paper of DuPont does not clearly indicate to which extent the process integration and parts of the existing pulp and paper mill are allocated to the system analyzed in the LCA. Since the presented LCA fully includes process integration, it can be assumed that the presented LCA yields higher impacts than the LCA of DuPont (DuPont 2012).

Furthermore, the LCA of DuPont uses primary data, while the presented LCA uses secondary data, as the process is still in the conceptual phase and thus not commercialized. This needs further investigation during the commercialization phase to optimize the flows and reduce the sustainability impact, as suggested in the previous section. Nonetheless, it can be concluded that process integration shows a significant effect on the sustainability potential. Furthermore, all three mentioned processes use lignocellulosic biomass as feedstock.

As a general conclusion, it is also important to point out that while the commonly regarded impact on greenhouse gas emissions for the xylitol biorefinery is marginal, other impacts are significantly higher, namely, freshwater ecotoxicity, marine ecotoxicity, and human carcinogenic toxicity. This is due to the use of electric energy from windmills induced by copper in the windmills. The mining of copper has a considerable impact on these impact categories, which translates directly into the results of the LCA of the biorefinery, despite wind energy being considered renewable and hence more sustainable due to its low impact on global warming. In order to reduce this impact directly, the use of other sources of electricity, e.g., solar or hydroelectricity, can be a solution, but this depends on the location of the plant and can possibly lead to other increased impacts in different categories. As a general conclusion, it can be stated that sustainable processes are a multi-layered issue, and a straightforward sustainable solution does not commonly exist; hence, further research on biorefinery concepts in the different impact categories is necessary.

Lastly, the presented analysis shows the importance of systematic LCAs for the sustainability assessment of processes. While the apparent lower impact on greenhouse gas emissions is visible, other priorly unexpected impacts can change the entire sustainability assessment of such processes. Hence, the systematic impacts of all processes are crucial to compare the improved sustainability impact to existing processes. Complementarily, the combination with a techno-economic assessment gives additional perspectives for decision-making on the overall feasibility and potential benefits of the investigated process (Grasa et al. 2021; Ögmundarson et al. 2020; Vollmer et al. 2022c). Particularly for novel biotechnological processes, or biorefineries, such comparisons allow for a quantified statement and assist the expedited transition towards genuinely sustainable processes, as postulated by the 2030 agenda for sustainable development of the United Nations (United Nations 2015).

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Data availability The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Competing interests The authors declare no competing interests.

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