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Environmental sustainability assessment of HMF and FDCA production from lignocellulosic biomass through life cycle assessment (LCA)

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Abstract: 2,5-Furandicarboxylic acid (FDCA) and 5-hydroxymethylfurfural (HMF) are top biomass-based platform chemicals with promising potential and an essential part of the future of green chemistry. HMF can be obtained mainly from fructose or glucose. Lignocellulosic glucose has a high production potential from not edible biomass. In the present paper life cycle assessment (LCA) was performed aiming at a better understanding of the environmental performance of the production of FDCA and HMF from lignocellulosic feedstock. Two case studies from the literature were modeled to obtain the life cycle inventory data. The production routes to FDCA comprise seven different process sections: hydrolysis, HMF synthesis, HMF recovery, FDCA synthesis, FDCA flash separation, FDCA purification and HMF boiler. By means of the LCA methodology, solvents such as dimethyl sulfoxide (DMSO) and dichloromethane (DCM), together with the energy demand, were found to be clear critical points in the process. Two scenarios were in focus: Scenario 1 considered the purification of FDCA through crystallization, whereas in Scenario 2 purification was performed through distillation.

Keywords: 2,5-furandicarboxylic acid (FDCA), 5-hydroxymethylfurfural (HMF), biopolymers, biorefinery, life cycle assessment (LCA), second generation biomass

Introduction

One approach to cope with the growing world population, resource depletion, raw material instability and climate change (CC) is to increase the production of chemicals from sustainable biomass-based products. To this end, biorefinery concepts are on the rise and it is valuable to evaluate their supply chain with regard to long-term environmental sustainability. The European Commission, for instance, provided a compilation of 94 bioproducts (fuels, chemicals and polymers) made from sugars, most of which are in the research and development stage (E4tech et al. 2015). In this context, life cycle assessment (LCA) is an important tool for the evaluation of a product or a production chain. In Europe, the “Bioeconomy Strategy” (European Commission 2018) was launched as an action plan to guide the European Union towards the application of sustainable resources. The European Standard EN 16760 (European Committee for Standardization (CEN) 2015) was also formulated as a help for good LCA practice for bio-based products.

According to the US Department of Energy, the biomass-based compound 2,5-furandicarboxylic acid (FDCA) is one of the 12 uppermost chemical building blocks. FDCA can be used for the production of polymers and resins and is often referred to as “the sleeping giant” as it can replace the fossil-based terephthalic acid for the creation of novel products (Wang et al. 2017). Polyethylene furanoate (PEF), for instance, is considered to be the “biopolymer of the future”, which can perform as a substitute for polyethylene-terephthalate (PET) (Papageorgiou et al. 2016) reducing the non-renewable energy (NREU) need from 51% to 43%, and the greenhouse gas (GHG) emissions from 54% to 46% (Eerhart et al. 2012).

Due to high costs, FDCA production is today at a niche level and only a few companies, mainly located in Europe, are involved in its manufacture. Currently, its production is dominated by the Dutch company Avantium.

Most efforts are directed towards FDCA production from 5-hydroxymethylfurfural (HMF), though it could also be produced from aldaric acids through dehydration and

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cyclization via acid catalysis (Miller et al. 2017). HMF is a furan derivative and an established basis for the production of a huge amount of chemicals (Torres et al. 2012). First generation feedstocks such as starch and cereal crops are the main source for HMF and FDCA production (Parshetti et al. 2015), but lignocellulosic biomass (second-generation feedstock), which does not compete with food and feed markets, can also be a source of HMF/FDCA. Lignocellulose consists of cellulose, hemicelluloses, and lignin, with cellulose being the most abundant carbohydrate on earth (Chen 2014).

The essential chemical steps for the formation of HMF and FDCA from hexoses are shown in Figure 1 and the technological routes of this process in are shown in Figure 2. Dehydration of C6 sugars yields HMF, subsequently, HMF oxidation and catalytic conversion produce FDCA (E4tech et al. 2015). Oxidation can proceed through autooxidation or aerobic oxidation (Lilga et al. 2010). Two pathways are viable: (1) heterogeneous catalysis with precious catalysts (Eyjolfsson et al. 2010) or non-precious metals catalysts (Lu et al. 2017), and (2) biotransformation with enzymes (Karich et al. 2018) or whole cells (Koopman et al. 2010). For the time being, the production of FDCA is

costly and polluting due to the high energy demand and the use of metal salts instead of environmentally friendly solvents (Koopman et al. 2010). In terms of cost and efficiency, the processing of C6 sugars into HMF as an intermediary product is more difficult than the route from HMF to FDCA (Grand View Research 2014).

The present study has its focus on the LCA of FDCA. The data of HMF production is based on the publication of Kougioumtzis et al. (2017), which uses sulfuric acid for acid hydrolysis, dimethyl sulfoxide (DMSO) for HMF synthesis, and dichloromethane (DCM) for HMF recovery. The HMF route towards FDCA is catalyzed by with a precious metal catalyst according to Triebel et al. (2013). LCA was already performed concerning the conversion of fructose biomass to biopolymer (Eerhart et al. 2012; Isola et al. 2017). However, there are no LCA studies available on FDCA production of glucose based on lignocellulosic materials. According to the ISO 14044 standard (2006), LCA can contribute to a better environmental performance of processes and products. As the FDCA production process is still in its infancy, the expectation is that the LCA will be helpful to the process development for FDCA production.

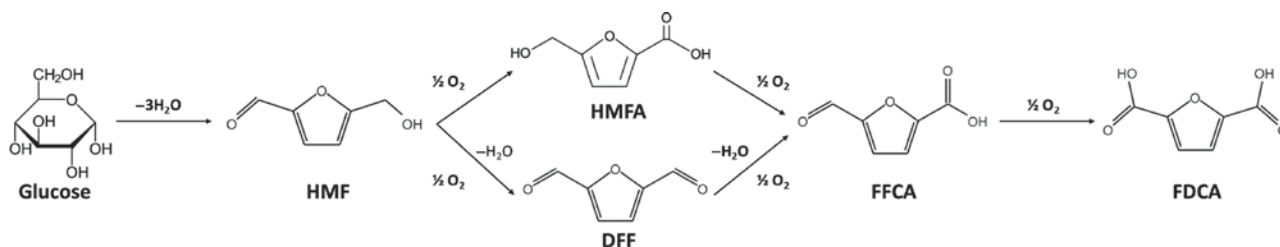


Figure 1: Essential conversion steps from hexoses to HMF and FDCA.

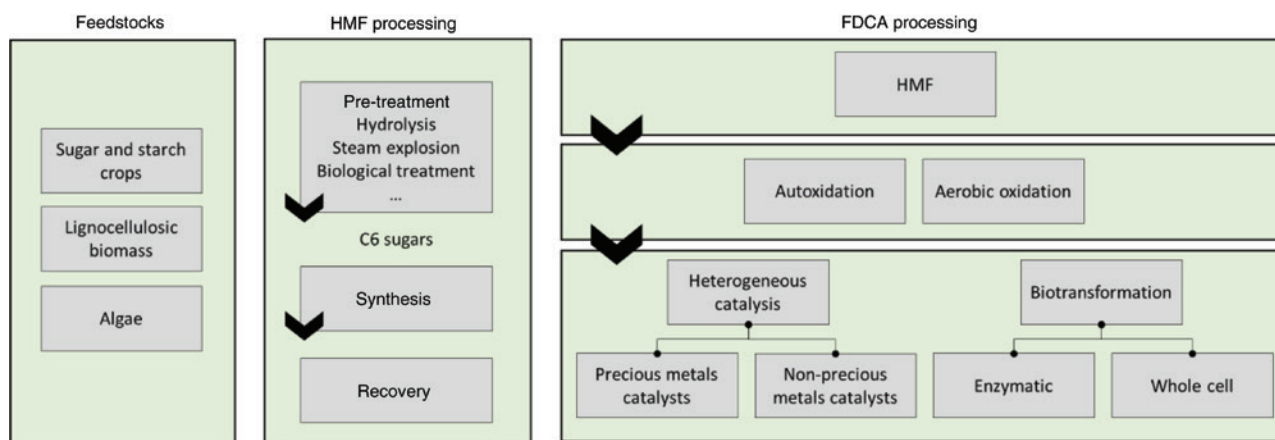


Figure 2: FDCA production pathways from different feedstocks through HMF.

Materials and methods

Basics of LCA: The LCA methodology (ISO 14040 2006; ISO 14044 2006) is a systematic tool used to determine the environmental hot-spots of a process or product along its value chain. Throughout the codes of practice that have addressed the recommended guidelines for LCA development (SETAC, ISO, ILCD handbook) there are common concepts and terminology. LCA, also known as eco-balance, aims to quantitatively relate each input and output of a clearly defined system with an environmental burden. It consists of four phases: goal and scope determination, inventory analysis, impact assessment and interpretation. The definition of the goal and scope aims to establish the boundaries of the study in terms of process, functionality, scope within the value chain, etc. The inventory analysis is one of the most time-consuming phases of the study and consists of the compilation of mass and energy data (inputs and outputs) of the process within the defined scope. The impact assessment phase is the stage at which every environmental burden related to an input or output of the process is assigned to a different environmental impact category depending on its nature (Klöppfer 1997). The impact categories of an LCA study are mainly provided by the used method (e.g. ReCiPe, CML, IMPACT2001). Each method differs in the characterization factors used for the assignment of environmental burdens. Some common impact categories are, for instance, ozone depletion (OD), climate change (CC) or terrestrial acidification (TA). The interpretation phase deals with the outcome that practitioners can obtain from the results of the study: decision making, government policy making, early improvement of novel processing technologies, etc. (Tecchio et al. 2016).

Goal and scope: In this work, the main objective is to assure the sustainable production of the combined route: biomass-HMF-FDCA. The functional unit of the LCA study was the production

of 1 kg of FDCA/h at the factory gate. The scope of the study was defined as a “cradle to gate”, taking into account the processes involved in the production of raw materials up to the final recovery of the purified FDCA. Due to the great versatility of the FDCA, sections of the value chain such as the use stage or final disposal were not considered.

Production system and system boundaries: The HMF production route in this assessment is a configuration involving triple dehydration of hydrolyzed glucose by catalytic synthesis. The production process of FDCA is based on heterogeneous catalysis with precious metals. Two scenarios will be considered: Scenario 1 includes a flash separation process after the reaction and the following steps of crystallization and filtration. Scenario 2 combines two flash separation processes and a distillation column. Kougioumtzis et al. (2017) studied the experimental and simulated process production of HMF via glucose transformation. Triebel et al. (2013) discussed the production of FDCA from HMF via process simulation work. These two papers served as basis for the present work, while the industrial feasibility was in focus. The Aspen Plus™ (Aspen Technology, Inc., Bedford, MA, USA) process simulator was used as technical aid. The FDCA production scheme has been segmented into seven subsystems (SS), which are explained below. The process flow diagrams for both scenarios, together with the representation of the system and subsystem boundaries, are presented in Figures 3 and 4.

SS1 hydrolysis: Hardwood chips, which are residues from forestry operations, undergo acid hydrolysis to obtain lignin, cellulose and hemicellulose fractions of wood and hydrolyze cellulose into glucose. The wood chips are mixed with sulfuric acid (0.75% wt) in aqueous solution at 175°C. After filtration for the elimination of residual solids (biotar), the stream is thermally treated to evaporate water and achieve a glucose concentration of 7.8% wt.

SS2 HMF synthesis: The glucose is converted to HMF in a catalytic reactor at 150°C and 8.2 bar. The catalyst is $\text{Sn}_2\text{O}_3\text{-}\gamma\text{-Al}_2\text{O}_3$, and

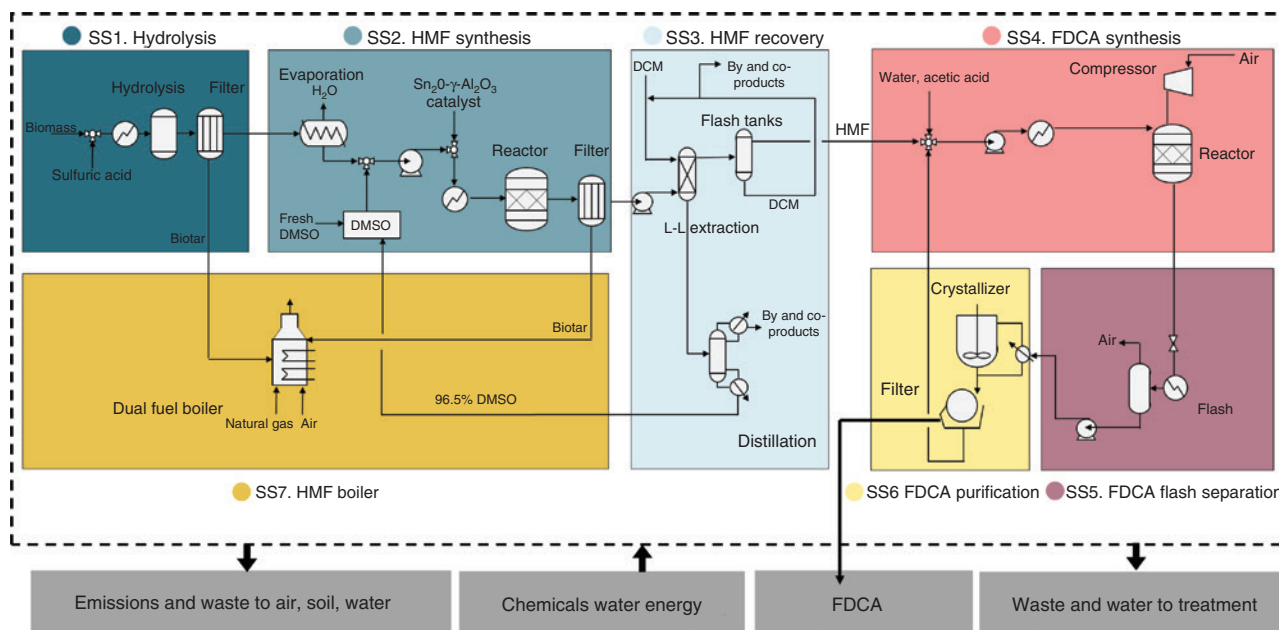


Figure 3: Process flow diagram and system boundaries for the production process of FDCA from HMF, Scenario 1.

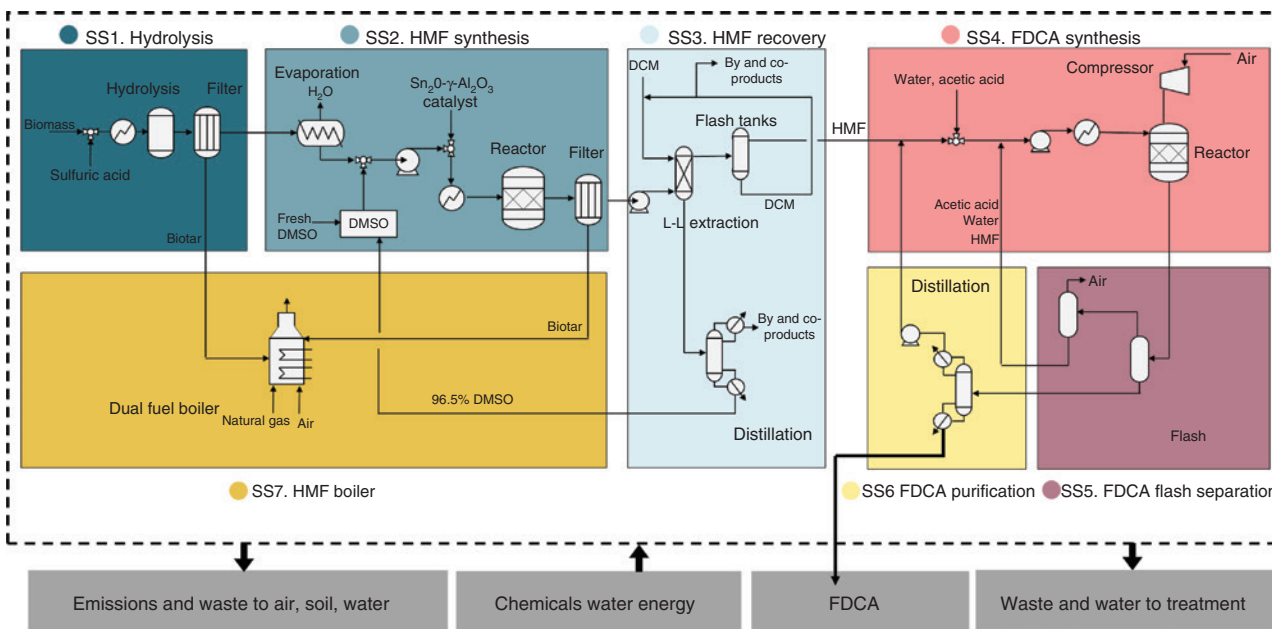


Figure 4: Process flow diagram and system boundaries for the production process of FDCA from HMF, Scenario 2.

DMSO/water (8/2) is used as solvent. The solution is filtered before the next processing steps.

SS3 HMF recovery: The final goal is a 96.5% HMF concentration. HMF is extracted from other reaction products with DCM/water (9/1) in a liquid-liquid extraction column. The DCM/water mixture is used in a quantity 10 times greater than the solution to be separated. For extraction, three flash separators are used with decreasing pressures (1, 0.8, and 0.1 bar). DCM is recirculated to the extraction column. The solution, which consists of by-products of the reaction, is treated in a distillation column to separate DMSO and recirculate it back to SS2.

SS4 FDCA synthesis: HMF (0.5%) enters the catalytic reactor together with an acetic acid solution (40%) at 100°C and 10 bar. The catalyst is Pt/ZrO₂. Oxygen is pressed into the reactor as excess air with a compressor.

SS5 FDCA flash separation: In Scenario 1, a single flash separator is used for the initial separation at 30°C and 1.5 bar. The output stream from the reactor is cooled in a heat exchanger in one step prior to the flash-drum. The main objective of the flash is the separation of air (mainly N₂ and O₂), which comes from the column top. The bottom stream is pumped into a crystallization unit working at 25°C. Scenario 2 includes two flash separator steps. The first one works at 100°C and 1 bar. The vapor phase, at the top, is a stream containing mainly water, acetic acid and air (N₂ and O₂). This stream is led to the next flash separator, which separates as much air as possible from the stream, to facilitate the recirculation of water and acetic acid to the reactor feed. The second flash separator operates at 37.5°C and 1 bar.

SS6 FDCA purification: In Scenario 1, the bottom flow of the flash separator (SS5) is pumped to a crystallization unit operating at 25°C. The crystallized FDCA is separated in a rotary vacuum filter as a solid, and the remaining solution is recirculated to the reactor feed. In Scenario 2, the bottom flow of the first flash separator (SS5) is directed to a distillation column operating at 0.55 bar. The product (FDCA) leaves the column through the bottom with a concentration

of 99.7%. The distillate contains mainly water and acetic acid is ready for reuse.

SS7 HMF boiler: The boiler provides energy exclusively to the HMF production subsystems (SS1, SS2, and SS3). It burns residual solids from the HMF production (biotar) and natural gas.

Life cycle inventory (LCI): Input and output inventories based on mass and energy balances of the bioproduction route are presented in Table 1 (Scenario 1) and Table 2 (Scenario 2). The inventories for the production of HMF have been adapted, as secondary data, from the work of Kougioumtzis et al. (2017). The data for the production of FDCA from HMF were evaluated by means of the simulation software in Aspen Plus™ based on an adaptation of the work of Triebel et al. (2013). Tables 1 and 2 present inventory data for the defined subsystems; in the case of HMF-related subsystems (SS1, SS2, SS3, SS7), inventory data are included taking into account the economic allocation of products, explained in more detailed below.

LCA methods: The ReCiPe 1.12 hierarchist method was applied (Goedkoop et al. 2009) and implemented via the SimaPro 8.02 software (PRé Sustainability, Amersfoort, The Netherlands). Impacts were determined up to the midpoint level categories as presented in Table 3. The selected impact categories from the ReCiPe method were considered to be the most relevant in case of biorefining processes. The vast majority of impact categories were described in the context of biomass transformation to biochemicals and/or biofuels (Collet et al. 2014; Lin et al. 2015; Gnansounou and Kenthorai Raman 2016; González-García et al. 2016).

Allocation: Economic allocation was considered for the Scenarios 1 and 2 related to HMF production (SS1–SS3 and SS7). The process is characterized by the production of other by-products and co-products that could be marketed. These streams depicted in Figures 2 and 3 contain a number of chemicals that can be recovered and sold.

Table 1: Inventory for the production of 1 kg/h of FDCA from HMF through the processing steps of Scenario 1 (purification through crystallization).

SS1 Hydrolysis		SS2 HMF synthesis	
Inputs		Inputs	
Biomass feedstock	3.06 kg	DMSO	0.58 kg
Water	27.57 kg	Sn20- γ -Al ₂ O ₃	1.35 · 10 ⁻⁵ kg
H ₂ SO ₄	0.21 kg	Electricity	0.87 kWh
Energy	7.76 · 10 ⁻³ kWh	Heating	3.9 kWh
		Outputs to technosphere	
		Wastewater	0.025 m ³
SS3 HMF recovery		SS4 FDCA synthesis	
Inputs		Inputs	
DCM	6.79 kg	Acetic acid	3.67 kg
Water	3.39 kg	Water	5.50 kg
Energy	4.8 · 10 ⁻³ kW	HMF	0.82 kg
HMF (96.5%) to SS4	65.85 kg	PtZrO ₂ catalyst	0.037 g
Outputs to technosphere		Electricity	15.83 kWh
Wastewater	22.10 m ³	Heating	14.08 kWh
		Cooling	1.40 kWh
SS5 Flash separation		SS6 FDCA purification	
Inputs		Inputs	
Cooling	11.97 kWh	Cooling	3.69 kWh
Electricity	0.017 kWh	Outputs to technosphere	
Outputs (emissions to air)		Wastewater	0.0088 m ³
Water	0.32 kg		
Acetic acid	0.23 kg		
Nitrogen	16.62 kg		
Oxygen	4.64 kg		
SS7 HMF boiler			
Inputs		Outputs	
Natural gas	0.63 kg	CO ₂ fossil	0.53 kg
Electricity	1.46 kW	CO ₂ biogenic	1.73 kg
Water	1.93 · 10 ³ kg		
Refrigerant R134a	Closed circuit		

For economic allocation, selling prices of the main marketable products were considered (Table 4). HMF was assumed to represent 16.4% of the total impacts of the production route.

Assumptions and limitations: The limitations of this environmental study are mainly due to the data quality of the inventories. These are based on secondary data (for subsystems related to HMF production) and simulated data (for subsystems related to FDCA production). In addition, this environmental study focuses on a techno-economically viable route. Another constraint is the accounting of biogenic CO₂, which remains a controversial issue among researchers, as there is a lack of a robust standard and criteria for its calculation (Liu et al. 2017). The components of emissions to air are negligible in quantity, such as the intermediates of the route HMF to FDCA (FFCA or DFF) were not taken into account. Concerning the catalyst Sn20- γ -Al₂O₃ for the production of HMF, a lifetime of 5 years was assumed. The

catalyst for FDCA production, Pt-ZrO₂, was assumed to have 10 years lifetime (Hidalgo et al. 2014).

Results and discussion

Environmental results in Scenario 1

The environmental profile of both scenarios allows for a comparative assessment of alternatives in relation to the downstream section of the process. The two different production pathways leading to FDCA have been analyzed by LCA. Figure 5 depicts the environmental impacts as

Table 2: Inventory for the production of 1 kg h⁻¹ of FDCA from HMF through the processing steps of Scenario 2 (purification through distillation).

SS1 Hydrolysis		SS2 HMF synthesis	
Inputs		Inputs	
Biomass feedstock	3.06 kg	DMSO	0.58 kg
Water	27.57 kg	Sn20- γ -Al ₂ O ₃	1.35 · 10 ⁻⁵ kg
H ₂ SO ₄	0.21 kg	Electricity	0.87 kWh
Energy	7.76 · 10 ⁻³ kWh	Heating	3.9 kWh
		Outputs to technosphere	
		Wastewater	0.025 m ³
SS3 HMF recovery		SS4 FDCA synthesis	
Inputs		Inputs	
DCM	6.79 kg	Acetic acid	3.92 kg
Water	3.39 kg	Water	5.88 kg
Energy	4.8 · 10 ⁻³ kW	HMF	0.82 kg
HMF (96.5%) to SS4	65.85 kg	Pt-ZrO ₂	0.039 g
Outputs to technosphere		Electricity	10.87 kWh
Wastewater	22.10 m ³	Heating	8.92 kWh
		Cooling	1.98 kWh
SS5 Flash separation		SS6 FDCA purification	
Inputs		Inputs	
Cooling	65.26 kWh	Cooling	8.42 kWh
Electricity	74.47 kWh	Heating	8.24 kWh
Outputs to technosphere		Electricity	1.14 · 10 ⁻³ kWh
Emissions to air		Outputs to technosphere	
Water	0.81 kg	Emissions to air	
Acetic acid	0.33 kg	Water	0.012 kg
Nitrogen	17.57 kg	Acetic acid	0.0083 kg
Oxygen	5.02 kg	Nitrogen	8.86 · 10 ⁻⁴ Kg
Wastewater	7.99 · 10 ⁻³ m ³	Oxygen	2.79 · 10 ⁻⁴ kg
		Wastewater	0.0088 m ³
SS7 HMF boiler			
Inputs		Outputs	
Natural gas	0.63 kg	CO ₂ fossil	0.53 kg
Electricity	1.46 kW	CO ₂ biogenic	1.73 kg
Water	1.93 · 10 ³ kg		
Refrigerant R134a	Closed circuit		

Table 3: Impact categories at midpoint level for ReCiPe 1.12 hierarchist method.

Impact category	Acronym	Units
Climate change	CC	kg CO ₂ to air
Ozone depletion	OD	kg CFC-11 air
Terrestrial acidification	TA	kg SO ₂ to air
Freshwater eutrophication	FE	kg P to fresh-water
Marine eutrophication	ME	kg N to marine water
Human toxicity	HT	kg 14 DCB to urban air
Photochemical oxidant formation	POF	kg NMVOC to urban air
Freshwater ecotoxicity	FET	kg 14 DCB to freshwater
Marine ecotoxicity	MET	kg 14 DCB to marine water
Agric. land occupation	ALO	m ² a
Fossil depletion	FD	kg oil

relative contributions for Scenario 1 (FDCA purification by crystallization). This scenario clearly illustrates that HMF recovery (SS3) and FDCA flash separation (SS5) are the major contributors to global impacts. Subsystem 3 (SS3) is the largest contributor to impacts in five of the 11 impact categories. Moreover, SS5 shows the highest shares in four of the 11 categories.

CC is affected mainly by SS3 and SS5, with 47.1 and 32.6% contributions, respectively. FDCA crystallization (SS6) has a contribution of 8.5% and FDCA synthesis (SS4) has a minimum contribution to the total CO₂ eq per kg. In terms of the high SS3 contributions to CC, DCM seems to be responsible with approx. 50% contribution for most of the categories. DCM is a volatile organic compound (VOC) widely used in industry as a solvent. It is also a

Table 4: Economic value of potentially marketable products and economic allocation factors.

Products	Econom. value (€ h ⁻¹)	Allocation factor (%)	Sources for market price of chemicals
HMF	110.31	16.4	(Mukherjee et al. 2015)
Acetic acid	17.25	2.6	(Himmelblau and Riggs 2004; Zhu and Jones 2009; Straathof and Bampouli 2017; ICIS 2018)
Formic acid	26.89	4.0	(ICIS 2018)
Fructose	0.84	0.1	(Mukherjee et al. 2015)
Lactic acid	53.17	7.9	(ICIS 2018)
Levulinic acid	14.93	2.2	(Mukherjee et al. 2015)
Mannitol	6.46	1.0	(ICIS 2018)
Hemicelluloses	1.07	0.2	(Persson et al. 2007; Li et al. 2013; Stoklosa and Hodge 2014)
Propionic acid	1.24	0.2	(ICIS 2018)
Lignin	422.22	63.0	(Hodásová et al. 2015; Budzinski and Nitzsche 2016; Nitzsche et al. 2016; Schwiderski and Kruse 2016; Zhao et al. 2017).
Glucose	16.30	2.4	(Heinzle et al. 2006; Klein-Marcuschamer et al. 2012)

carcinogenic chemical (Guo et al. 2004) and potential contributor to air pollution (Kikuchi et al. 2011). In fact, DCM is responsible for OD (Huang et al. 2014) as also seen in Figure 5, where SS3 represents a 99.3% contribution to OD.

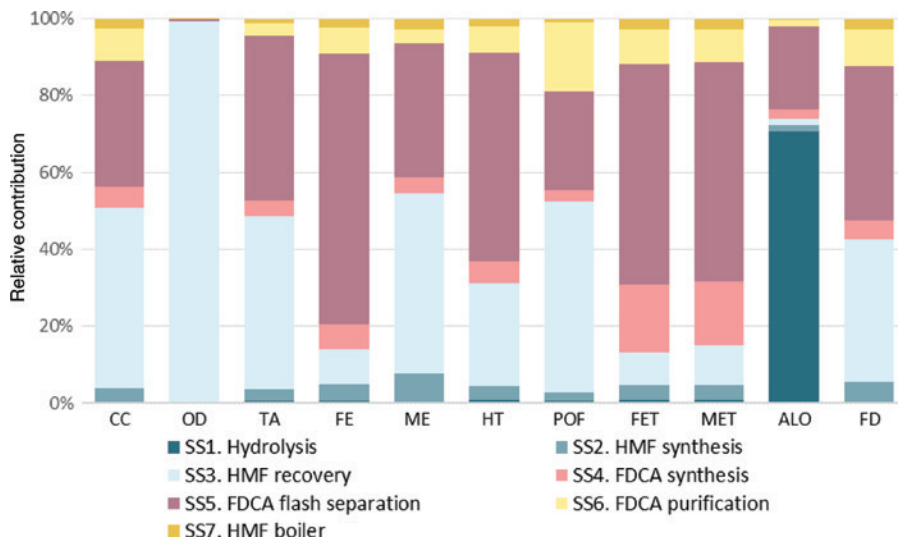
There are studies concerning the use of green solvents for HMF production instead of DCM (Yu et al. 2018). An option is the efficient γ -valerolactone (GVL) (Alonso et al. 2013), which can be derived from biomass and has a potential to improve environmental sustainability (Fegyverneki et al. 2010; Yan et al. 2015). For agricultural land occupation (ALO), as expected, 70.8% is due to hydrolysis (SS1), which includes aspects of land use related to forestry activities for the production of hardwood chips.

The most representative impacts of the SS5 are due to the flash separations carried out in the subsystem. The

flash separation operates at 1.5 bar because cooling is required in the output flow of the FDCA synthesis reactor. The exit flow of the reactor for the synthesis of FDCA (SS4) is at 10 bar and 100°C, making the separation step (SS5) prior to crystallization very energy consuming.

Environmental results in Scenario 2

Figure 6 shows the most relevant impact contributions to scenario 2 (FDCA purification by distillation). The distribution of impact contributions between subsystems tends to change slightly with some redistribution of impact. HMF recovery (SS3) continues to be a relevant contributor to all impact categories in the range of 1% (ALO) to 98% (OD) due to the use of DCM.

**Figure 5:** Process relative contributions (in %) per subsystem to obtain 1 kg h⁻¹ of FDCA (Scenario 1: Crystallization).

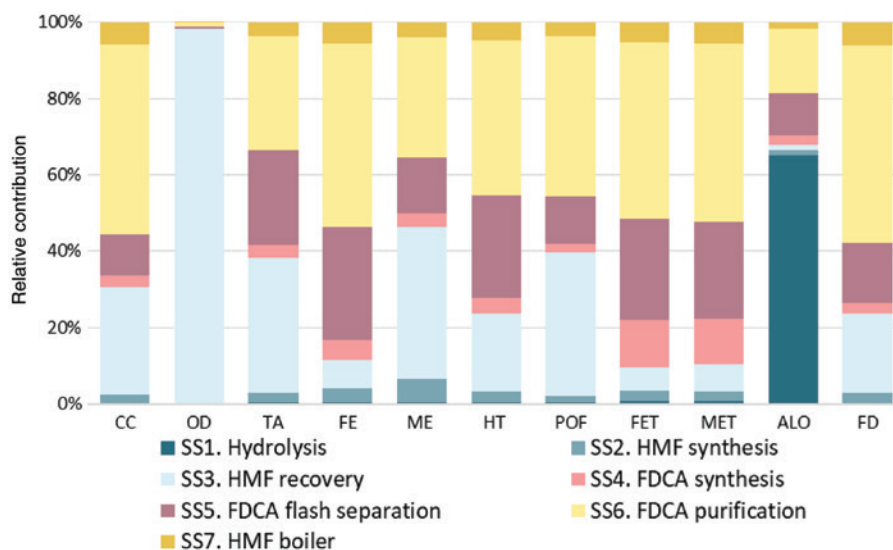


Figure 6: Process relative contributions (in %) per subsystem to obtain 1 kg h⁻¹ of FDCA (Scenario 2: Distillation).

The FDCA purification and separation subsystem (SS6) in Scenario 2 is a significant contributor to all subsystems (unlike in Scenario 1), being even more relevant than SS3. In six of the 11 impact categories, SS6 is the largest contributor with relative contributions of 50% CC, 48% FE, 42% photochemical oxidant formation (POF), 46% FET, 47% marine ecotoxicity (MET), and 52% FD. SS5, which is one of the most relevant contributors to environmental burdens in Scenario 1, is displaced by SS6 in Scenario 2 due to its high energy demand. In Scenario 2, the separation train includes a vacuum distillation column as well as flash separators for a better efficiency of feed materials (acetic acid, water, HMF) through recirculation. In Scenario 2, ALO presents the highest contributions from SS1, which is related to land occupation arising from forestry biomass production.

Chen et al. (2016) addressed the LCA of the production of PEF bottles and found that this process has a lower global warming potential than the fossil alternative as well as the improvement in OD and toxicity categories. The quoted and the present study show viable production routes in the context of biorefining. Isola et al. (2017) discussed the environmental assessment of the production of a photodegradable polymeric material. The production route was based on the synthesis of FDCA from HMF. In this case, HMF was derived from a fructose source rather than from glucose. The LCA showed that the fossil fuel chemicals (N,N-dimethylacetamide and lithium bromide, H₂SO₄, DCM) and energy consumption are the main hot-spots of the processing steps. FDCA and HMF are top bio-chemicals which offer numerous opportunities for the

manufacture of chemicals and materials; however, they present barriers such as low reaction yields and the need for non-renewable solvents and chemicals in large quantities for their production (Deneyer et al. 2018).

Environmental comparison of scenarios

Figure 7 illustrates the total relative contribution of each scenario. It is evident that Scenario 2 presents 25% worse results than Scenario 1. This is due to the high energy demand for distillation of FDCA in SS6, which is not offset by the environmental impacts in Scenario 1. However, OD is slightly different by 1%, as DCM is an ozone-depleting gas and its concentration and fate are the same in both scenarios. In contrast, fossil depletion (FD) is the main contributor to all environmental impacts in Scenario 2, with a 44% increment compared to Scenario 1, which is mainly due to energy consumption.

The ALO impact category shows greater impacts in the hydrolysis subsystem (SS1) for both scenarios due to forestry operations. Although this ALO impact category does not contribute significantly to the overall environmental assessment, land use is an important factor to be considered, particularly from the point of view of long-term application. An inappropriate land management may have very negative side effects, which are difficult to quantify, for example, concerning soil fertility, carbon loss and biodiversity loss, etc.

Due to its energy-intensive nature, the FDCA flash separation subsystem (SS5) has a major impact on

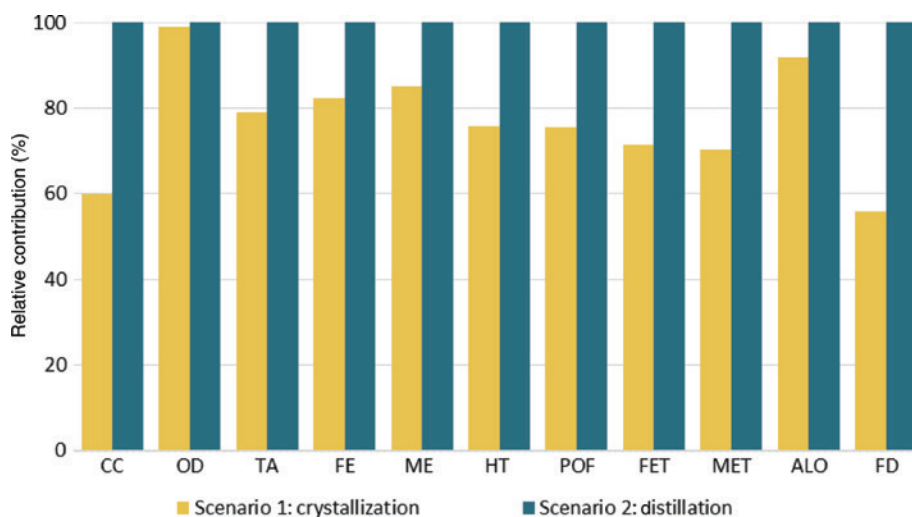


Figure 7: Comparative environmental profiles (in %) for Scenarios 1 and 2.

Scenario 1. However, the reconfiguration of the purification scheme substantially reduced this impact, converting the FDCA purification and separation subsystem (SS6) into the largest contributor among all impact categories in Scenario 2, again due to the high energy demand. The total environmental assessment clearly demonstrates that Scenario 1 is more sustainable.

Conclusions and future perspectives

The production of biochemicals and biofuels through the biorefinery route from lignocellulosic materials has been a relevant topic of discussion in recent years. The transformation of biomass into chemicals or biofuels has been studied, depending on the process, mainly in the laboratory or on a pilot scale, while optimization and scaling up to industrial scale are still in their infancy. In the present study the potential production route for FDCA was assessed for a larger scale production to fill the gap in terms of environmental feasibility of such processes. LCA is a useful tool to consider regarding sustainability and environmental performance. However, the environmental sustainability of these processes is almost always hampered by the use of catalysts and solvents. Biomass-based chemicals do not necessarily contribute to environmental sustainability. HMF and FDCA production still need conventional solvents such as DCM, which harm health and the environment. In Scenarios 1 and 2, the HMF recovery subsystem (SS3) has a considerable impact due to the use of DCM. Therefore, the research on FDCA production should be extended to the use of more environmentally friendly substances. Lowering the energy

requirements should also be studied. The LCA results of the presented research can be considered as aids towards further improvement of the biorefinery concept.

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