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Towards improving the sustainability of bioplastics: Process modelling and life cycle assessment of two separation routes for 2,5-furandicarboxylic acid

Sara Bello*, Pedro Méndez-Trelles, Eva Rodil, Gumersindo Feijoo, Maria Teresa Moreira

Department of Chemical Engineering, Universidade de Santiago de Compostela

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ABSTRACT

Within the framework of an economy excessively dependent on fossil resources, the concept of sustainable development, aimed at obtaining environmentally friendly consumer goods, has given rise to the development of biorefineries. These facilities are based on the production of biofuels and platform chemicals from the most abundant raw material on the planet: biomass. The use of biomass such as wood or lignocellulosic residues makes it possible to seize opportunities offered by the implementation of renewable feedstocks, which in many cases can be embedded within the perspective of circular economy, through the exploitation of residual fractions. Among the multiple basic chemicals that can be obtained from biomass, 2,5-furandicarboxylic acid (FDCA) has a great potential, as it is the precursor of poly(ethylene furanoate) (PEF) polymer, which is considered a feasible substitute for poly(ethylene terephthalate) (PET). The purpose of this study is the simulation and environmental analysis of two separation routes for FDCA production with the objective of identifying the environmental hotspots at an early stage of the process design. The present study addresses the modelling of FDCA production from hydroxymethyl furfural (HMF) by heterogeneous catalysis using commercial Aspen Plus® V9 software. Two different downstream separation options resulting in purified FDCA were simulated: crystallization (Scenario A) and distillation (Scenario B). The estimation of the mass and energy balances were considered in the development of the data inventories required to conduct Life Cycle Assessment (LCA). LCA-assisted decision making identifies the conceptual configuration that would eventually lead to the least environmental burden. In the case of Scenario A, the stage with the highest environmental burden was the reaction unit, due to the use of HMF. In Scenario B, on the other hand, the separation stages contributed most to the impact due to their high energy demand. The combination of process simulation and LCA allowed acquiring a detailed vision of the process, through the analysis of the sensitivity of the environmental profile to different process parameters. The operating pressure in flash and distillation units for both scenarios affects plant operation by influencing total energy consumption and FDCA production. The sensitivity of environmental outcomes to these parameters was also studied, resulting in small variations. Thus, the results of this assessment provide strategic information of the early decision-making process on potential configurations for industrial-scale FDCA production.

1. Introduction

So far, the production of 2,5-furandicarboxylic acid (FDCA) has been performed through the use of heterogeneous chemical catalysts [1,2]. The growing interest in the search of different ways of producing FDCA from biomass is justified by its great potential to replace petroleum-based chemicals. This top platform chemical [3] will clearly undercut the use of non-renewable raw materials for the production of, for instance, plastic bottles, textiles or coatings [4]. Poly(ethylene furanoate) (PEF) is the polymer that can be obtained from FDCA, which is renewable and achieves better mechanical properties than its fossil counterpart poly(ethylene terephthalate) (PET). The production of PEF compared to PET is expected to experience a marked reduction in the environmental impacts [4,5]. In recent years, there has been a proliferation of studies attempting the enzymatic conversion of hydroxymethyl furfural (HMF) to FDCA [6–8]. In both cases, yields and conditions are not considered optimal for realistic, large-scale production and therefore the main concern with respect to FDCA production is that production expectations may not be met. On the other hand, to the knowledge of the authors, there are almost no studies that evaluate any of these production routes under an environmental perspective [9–11].

Biomass has always been available for the production of energy and

* Corresponding author.
E-mail address: sara.bello.ould-amer@usc.es (S. Bello).

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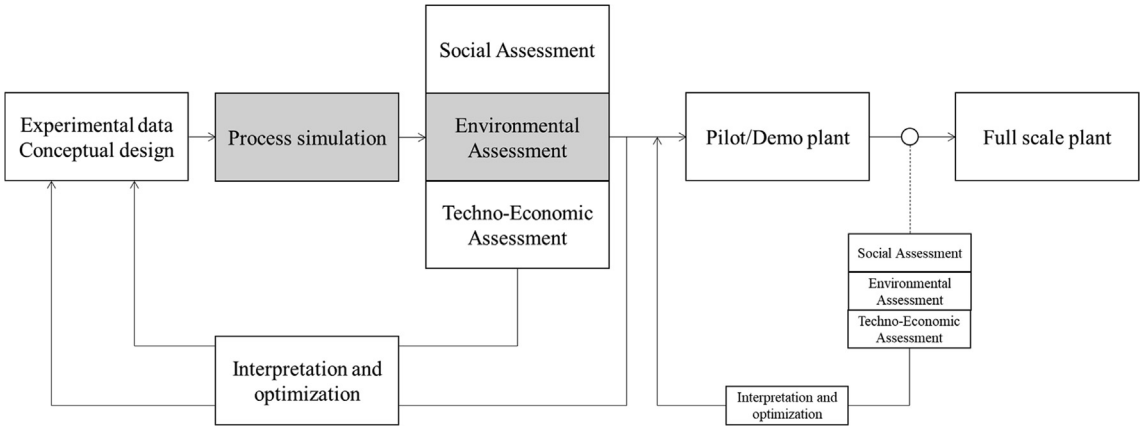

Fig. 1. Framework for the design and projection of new production routes. The phases included in the scope of this work are highlighted in grey.

materials, but its importance endured a less relevant status when, at the end of the 19th century, oil reserves started to be exploited as a direct consequence of the Industrial Revolution [12]. However, today, with fossil fuel reserves declining at a high rate due to the inverse proportional increase in population, the secondary role of biomass is very likely to change in the coming years. Biomass can be considered mostly as organic matter, classified as woody biomass, herbaceous and agricultural biomass, aquatic plants, animal and human biomass wastes, contaminated biomass and industrial wastes [13]. For instance, although the production of platform chemicals and materials is not considered, it was estimated that the global demand for primary energy (2012) was around 500 EJ/year, which could be supplied exclusively from biogenic sources [14]. Lignocellulosic biomass is a renewable raw material that provides a good platform to support society's current economy. On the other hand, the valorization of lignocellulosic residues which would otherwise have to be managed offers a perspective of circular economy [15]. However, the use of biomass as raw material, and more specifically lignocellulosic biomass, is not exempt from a number of limitations. First, the technology needed for pretreatment and production of biochemicals has not yet matured. This has an effect on the production cost of these kinds of products, which is remarkably high when compared with traditional production routes. On the other hand, the intricate morphological structure of wood heightens the above-mentioned challenges [16].

On a separate note, the industry has always sought to improve process productivity and, therefore, its competitiveness in the market. With the development and evolution of computational tools, industrial process analysis strategies have evolved drastically in recent years. Process simulation conveys several advantages, such as the possibility of estimating results based on process variables and technical data from the system under study [17]. In this context, Aspen Plus® is a software package specially developed for simulating chemical process models relieving the user from performing complex calculations. It enables process optimization, improving competitiveness, reducing costs and unplanned downtime. This process simulation package has been used to model several processes based on the use of biomass as feedstock for the production of biofuels and biochemicals [18–20].

Governmental bodies in Europe have set targets through multiple initiatives for bio-economy that can be grouped into three main objectives defined as achieving low carbon processes, optimizing the use of raw materials and resources through efficient technologies, and establishing a competitive niche for bioproducts in the market [21]. Our work has considerably considered the established objectives. The evaluation of a process through environmental assessment, such as Life Cycle Assessment (LCA), should help to determine what the critical points are in relation to the environmental aspects and how to tackle them correctly. Resource efficiency involves the disposition and availability of biomass raw materials; the potential problem of availability may be a bottleneck in the value chain of a product, but research on ways to exploit more residual-type streams (wood and agriculture residues, urban waste, etc.), taking into account circular economy issues, should ensure a better disposition of resources. Finally, market competitiveness can be achieved with a fully optimized process and through the manufacture of a product such as FDCA, which has the potential to be highly valued among other bio-based products.

LCA has been considered as an effective methodology allowing to evaluate and benchmark, from the environmental perspective, different alternatives to determine the best possible solution. Not only does LCA provide a framework for environmental evaluation, but also a platform for holistically assessing any process or product from the perspective of the value chain and circular economy issues [22].

The aim of this work is to comparatively assess the environmental implications of two different separation routes. Separation processes are known to be economically demanding, not only in bioprocessing but also in conventional production routes. For the most part, this is due to their energy intensive characteristics, which is a challenge that is definitely tied to the environmental performance of any configuration. Furthermore, separation processes in biorefineries are challenging in many cases due to the dilution of the product in the streams, inhibitory effects or the need of separation in water-based streams [23]. The objective of the present work is to combine process simulation with ex-ante LCA to support the sustainable conceptual design of an FDCA production route. It is, in fact, not unusual to present the eco-design of processes through the coupling of process simulation and LCA [24].

2. Materials and methods

The key evaluations of an industrial project are usually those related to techno-economic, environmental and social aspects, which help to provide an overall overview. The outcomes of the assessment of the projected facility may provide insight on ways to optimize the process with feedback to the starting point for design improvement. The main aspiration of this study is to execute part of the framework for the design and projection of new production routes, as those shown in Fig. 1, providing an overview of the environmental aspects and a proposal of opportunities for process improvement.

When considering a systematic approach for the design of future biorefineries and other processing facilities, it is common to implement an iterative procedure considering the numerous possibilities within their development. Firstly, the project design normally begins with experimental laboratory research on the chemical reactions and physical processes involved in the transformation route under consideration (thermodynamic properties, reaction kinetics, etc.). Once experimental data and a preliminary conceptual design are available, the first approximation to process simulation can be performed. Process simulation aids to simultaneously evaluate the numerous degrees of freedom

existing when designing a process with multiple process units. The outputs of a process simulation are a series of mass and energy balances, stream properties and equipment working conditions. Preliminary data obtained from a simulation can be used for the early environmental assessment of the plant.

2.1. General description of the process

The oxidation of HMF to FDCA has been examined by the scientific patent for hydroxymethyl furfural oxidation [25]. The chemical transformation of HMF to FDCA, according to the patent, can be performed through the oxidation with the use of air and a solid metal catalyst (platinum) supported on ZrO_2. In a fixed bed continuous reactor, the HMF feedstock is added in a ratio of 0.5% wt. to an acidic aqueous solution (acetic acid solution in water, 40:60).

Triebl et al. [1] proposed the same transformation of HMF to FDCA and its separation through two different procedures. In the first case, the authors considered an approach involving the separation of FDCA through a crystallization unit and filter, from this point forward, Scenario A. The second approach was based on the separation of the components with the use of a liquid-liquid extraction unit and subsequent distillation for the recovery of the extractant, hereafter Scenario B. However, in the case of this study, a critical evaluation of the proposed configurations has been contemplated. The first modification of Scenario A was the simplification of the process by eliminating air recirculation. It was considered that the energy demand for the compressing power to perform air recirculation was not essential considering the amount of residual O_2 released. On the other hand, the high content of inert (N_2) in the air recirculation requires a larger volume of the plant, even if there is a purge. However, due to the high boiling points of both compounds, the energy consumption of the separation is expected to be high. This leads to the possibility of exploring vacuum distillation, which would allow working at lower temperatures. From an environmental point of view, this approach aims to reduce the high toxicity values of the use of organic solvents such as trioctylamine. The European Regulation on Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) of the European Chemicals Agency (ECHA) [26] has determined that trioctylamine is very toxic to aquatic ecosystems and humans. In the case of air recirculation [1], it has been avoided, once again, in the new configuration for Scenario B. The generalized block diagram for the production process under consideration is provided in Fig. 2. A more detailed explanation on the simulation arrangement for both cases is given in Section 2.2.

2.2. Aspen Plus® modelling approach

The Aspen Plus® V9 process simulator was the commercial software selected to model the FDCA production and separation route according to the conditions defined in the previous section [1,25]. The modelling

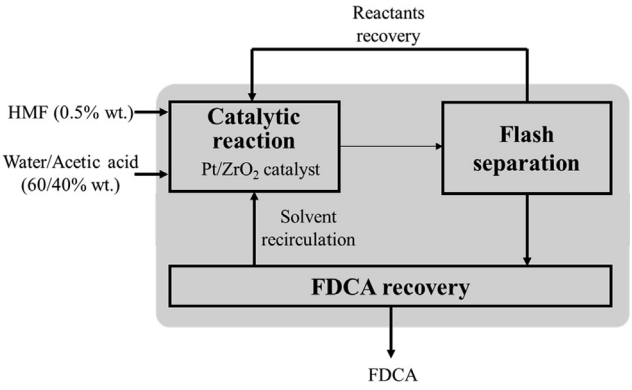

Fig. 2. Process block diagram for the catalytic production of FDCA from HMF.

of the upstream section of the configuration is common to both case studies. The definition of the input flow was made according to the specified composition required for the reaction mechanism. Fresh water, acetic acid, HMF and air are the inputs to the system, which enter the process at ambient temperature and pressure, 25 °C and 1 bar. The input streams must be conditioned to reach the operating temperature and pressure of the reactor, which are 10 bar and 100 °C. The pressure increase of the liquid stream is carried out with a pump, while the air is introduced into the reactor with a 3-stage isentropic compressor with a discharge pressure and a temperature of 10 bar and 100 °C respectively. The discharge pressure of the pump is also 10 bar, and then a heat exchanger raises the temperature of the liquid stream to the required value of 100 °C.

It is key to ensure the reaction conditions and compositions that will enter the reactor due to the nature of the block selected to model the reactions. A stoichiometric reactor block functions as a black box model, basing the calculations for the output products on the specified yields achieved under specific temperature and pressure values. It was considered that impurities in the reactor (co-products and by-products) do not affect the performance of the reaction.

Considering the reaction mechanism depicted in Fig. 3, yields are 90% for FDCA production from HMF, 2% for 2,5-diformylfuran (DFF) production, 0.5% for 5-formyl-2-furancarboxylic acid (FFCA) production, 10% for FDCA production from FFCA and 10% for FDCA production from DFF. FDCA is supposed to be obtained through the reaction pathway of DFF [25]. Unlike the upstream section, which is equivalent for both scenarios, the downstream differs attending to the case of study. The separation sequence applied to the reactor output stream is detailed in Sections 2.2.1 and 2.2.2.

2.2.1. Scenario A: FDCA production and recovery by crystallization

Fig. 4 depicts the flowchart developed for Scenario A. In Scenario A, the separation sequence starts with an expansion valve working at a discharge pressure of 3.5 bar. The objective is to condition the output flow of the reactor (stream 7) to milder conditions, i.e., closer to ambient pressure and temperature. Heat exchanger E-2 contributes to the same purpose, aiming at an output temperature in stream 9 of 30 °C. The adiabatic flash unit F-1 has the function of performing liquid-vapor separation at. The vapor stream exits the unit with a composition rich in air and steam, along with residual acetic acid fractions. Most of the air (89% of the input stream) is removed through the vapor stream 10. The liquid stream (stream 11) is pumped to the crystallizer with P-2. In the crystallizer, at 2.5 bar and 25 °C, the $FDCA^{-2}$ anion and H^+ yield FDCA. The solid product (stream 17) is separated with a 98% wt. solid fraction in the filter cake using the rotatory vacuum filter FI-1. The filtrate (stream 14) is recirculated and mixed with the feed stream (stream 1), a purge of 5% of this stream is included to prevent inert accumulation throughout the system (stream 16).

A design specification and a balance variable have been included in block M-1 to assist in the appropriate convergence of the model. Through these flowsheeting specifications, the model is able to update the flow of the make-up stream in the recycle calculations. The HMF concentration at the reactor inlet was set at 0.5% wt. through the design specification.

2.2.2. Scenario B: FDCA production and recovery by vacuum distillation

Fig. 5 depicts the flowchart developed for Scenario B. In the case of Scenario B, the first unit operation after reactor R-1 is flash F-1. This unit operates at 100 °C, decreasing the output pressure of 10 bar from the reactor outlet to 1 bar. The objective of F-1 is to separate in the vapor phase as many of the most volatile components in stream 9. The separated vapor stream (stream 10) exits through the top of the unit containing mainly water, acetic acid and air (as O_2 and N_2). The liquid fraction contains the target product (FDCA) and other by-products and chemicals (water, acetic acid, HMF, DFF and FFCA). Reducing the working pressure and volume of the flow to be treated in the

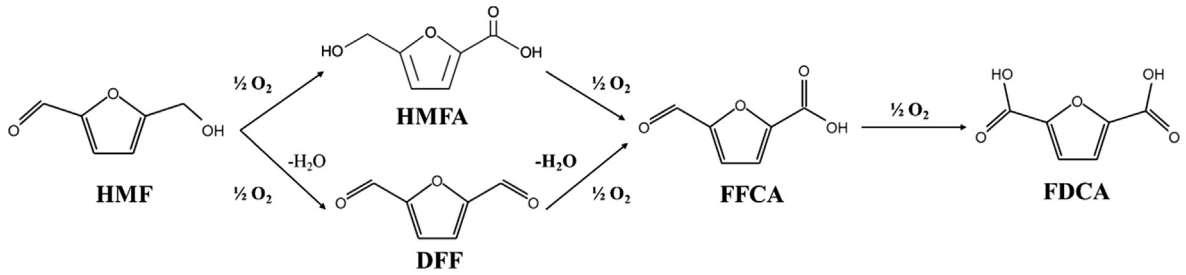

Fig. 3. Mechanism of HMF oxidation to FDCA. Adapted from Lolli et al. [27].

downstream separation unit will reduce energy requirements. Stream 11 continues to the vacuum distillation column D-1, which works at 0.55 bar. The boiling point of the compounds would imply an intensive energetic demand for their separation (FDCA: 420 °C). Reducing the working pressure by applying vacuum distillation lowers the boiling point of the compounds. The vacuum distillation column selected was a DSTWU block with a total condenser and 10 stages. HMF was set as the light key with a recovery of 0.99 and FDCA was set as the heavy key, with a recovery value of $1 \cdot 10^{-6}$. The energy demand required to decrease the operation pressure to vacuum values would be reached through the used of a vacuum pump. However, in this study, this energetic requirement was not considered. Stream 17 contains the final FDCA with a mass fraction of 99.7%. In this Scenario, streams 10 and 16 contain a mixture of air, water and acetic acid as main components. The objective is to recover the water and acetic acid and recirculate it to the reactor and, on the other hand, to remove air. This is performed through the F-2 (37.5 °C and 1 bar) and F-3 (81 °C and 1 bar) flash units respectively. The simulation included the purge of the recirculation streams in a ratio of 5% to prevent inert accumulation throughout the system.

In the same way as in the previous Scenario a design specification and a balance variable were included in block M-1 for the calculations of the recycle flows. Table 1 presents a compilation of Aspen Plus flowsheet unit operation blocks and conditions included in Scenarios A and B.

2.2.3. Thermodynamic model

The selection of the thermodynamic properties model, among the options available in the simulator, was performed with the algorithm proposed by Carlson [28]. In the case of crystallization (Scenario A involving $FDCA^{-2}$ and H^{+} ions), the Electrolyte NRTL model was used. In the case of vacuum distillation, Scenario B, the NRTL model was selected. For the estimation of the properties of the components involved, the simulator allows to directly introduce the components of its database, except for the reaction intermediates: DFF, FFCA and $FDCA^{-2}$, which were not available. Their properties were estimated according to their molecular structure, imported through files with extension (*mol*).

2.3. Aspen plus sensitivity analysis

The model presented includes the final variables and parameters used for the simulation of each Scenario. As a complement to the study, a sensitivity analysis of key parameters was performed with the support of the Aspen Plus Sensitivity Model Analysis Tool. Considering the degrees of freedom in the process simulation, there is a need to evaluate certain variables attending to the final objectives of the process. In this case, the overall objective was to minimize the energy consumption of the process units and maximize the purified FDCA obtained. Each parameter was evaluated in a single step and varied within the operation limits. The parameters analyzed were kept constant at their optimal value to evaluate the effect of the related variables. The sensitivity assessment focused mainly on downstream separation operations. The analyzed variables were the operating pressure at unit F-1 for Scenario A and the operating pressure of units F-1 and D-1 for Scenario B. These variables were analyzed in the range of feasible operation, with the ranges corresponding to minimum and maximum pressure. This range of operation has been retrieved from the limiting pressure values computed by the simulation without any errors in the flowsheet diagram. A constant increment was considered to obtain equidistant points in the selected range of operation.

2.4. Life cycle assessment methodology

This work presents a combination of process simulation work and environmental analysis of the simulation results to provide a forecast of the environmental implications within the processing routes studied. The Life Cycle Assessment (LCA) methodology is an approach that considers the interactions within the life cycle of a process or product that cause a burden on the environment. LCA methodology follows the guidelines set in ISO 14040 and ISO 14044 [29,30], that include four phases: goal and scope definition, Life Cycle Inventory (LCI), Life Cycle Impact Assessment (LCIA) and results interpretation (Fig. 6).

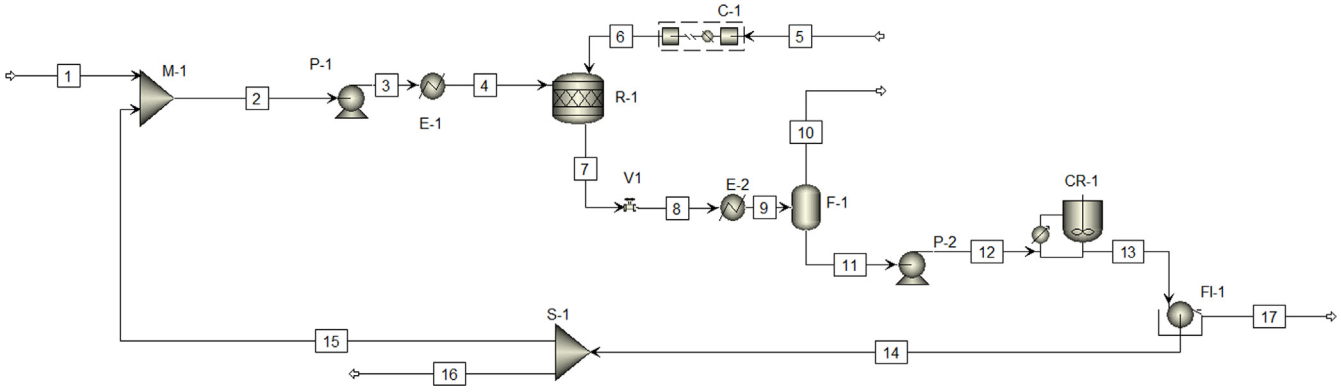

Fig. 4. Aspen Plus flowsheet for case A.

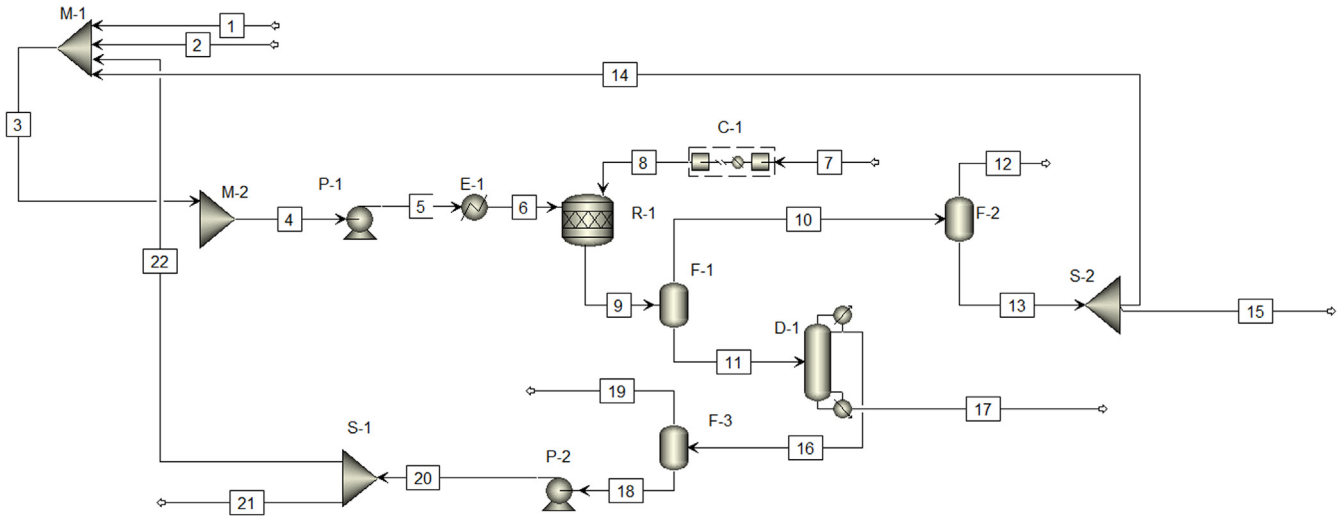

Fig. 5. Aspen Plus flowsheet for Scenario B.

2.4.1. Goal and scope definition

LCA is a useful tool which can support the identification of opportunities to improve the environmental performance of processes and products. In this case, the FDCA production process is still in its infancy and any effort to its optimization will lead to a better outcome. When it comes to novel processes, 'bio-' is not always synonymous of environmentally sustainable. The analysis of the processing route in this study through LCA aims to help in the determination of areas for improvement in order to guide efforts towards better environmental performance. The process analyzed is based on a chemical route for the production and recovery of the FDCA platform chemical. The separation operations within the production route may determine the limit at which the process can be considered environmentally sustainable. Thus, the objective of the LCA is to perform a comparative environmental assessment of two different schemes for the separation of FDCA obtained through a chemical route. On the other hand, the results of the Aspen Plus sensitivity analysis will be combined with the LCA methodology as a way of studying the influence of parameter selection on the environmental results. The functional unit is the calculation base that best represents the purpose of the system under study, in this case, the functional unit is the production of 1 kg/h of FDCA.

The system boundaries of the LCA study include the process units within the presented process simulation. The general overview of the LCA system boundaries is presented in Fig. 7. The process was divided into three subsystems for environmental analysis purposes. In both scenarios, Subsystem 1 (SS1) includes the catalytic reactor for the production of FDCA. Subsystem 2 (SS2) deals with the first flash units for the separation sequence. Finally, Subsystem 3 (SS3) includes the units for the final separation and purification of FDCA. In Scenario A, the crystallizer and the rotary vacuum filter are included within the subsystem boundaries. In Scenario B, the vacuum distillation unit is included within the system boundaries. The scope of the environmental study was considered to be a cradle-to-gate approach, which takes into account the impacts of the activities from the production, cultivation or extraction of raw materials up to the production of FDCA obtained.

2.4.2. Allocation, cut-off procedures and assumptions

The data considered for the environmental assessment is the data retrieved from the process simulation for the foreground processes. The inventories of most of the background activities were evaluated through the Ecoinvent 3.5 database processes [31]. Notwithstanding, the inventories used for the production of HMF could not be found in the database used. HMF is the main raw material used in the process and it is considered a very relevant but novel biochemical platform. Being part of the background processes for FDCA production, it is relevant to consider its impacts. Data for HMF production from lignocellulosic biomass was obtained from a peer-reviewed report [32]. Economic allocation was considered for the assignment of impacts to the main product (HMF) within the co-products and by-products obtained in the produced stream. Economic allocation was used in the case of HMF because, in the considered production process for HMF, the output stream is composed not only of HMF, but also of other co-products which are considered to have a potential market value (acetic acid, formic acid, lignin, fructose, etc.). Therefore, the impacts of the production process were not considered to be exclusively assigned to HMF [33].

Despite the possibility of retrieving mass and energy balance data from the process simulation, there are aspects of LCA that would depend on the implementation of the plant in a real industrial environment. Therefore, some assumptions were formulated. First, no transport activities were considered in the production of FDCA. In fact, it is considered that in a real site, HMF would be produced on site as part of the same value chain. Infrastructure, construction, installation or decommissioning processes were not considered for the FDCA production plant, since for this type of industrial facilities, due to their expected lifetime, their impact is generally considered negligible [34,35]. The hypothetical plant was considered to operate continuously 330 days a year. A lifetime of 10 years was considered for the metal catalyst and the quantity needed was calculated using the flow and the residence time of the reactor. The unavailability of the catalyst in the used database was overcome through the use of literature data, considering the use of platinum and zirconium oxide [25]. A catalyst bed density of 1300 kg/m^3 was assumed [36] along with the values of energy consumption during its production [37]. The catalyst quantity per functional unit was calculated considering the 10 years lifetime, therefore, the results per functional unit depict only the corresponding fraction of impacts before being substituted. The Spanish electric mix was considered when dealing with electricity consumptions throughout the FDCA production system. Moreover, the use of utilities was modeled environmentally by considering heating and cooling resources available in the Ecoinvent 3.5 database. A generic cooling energy source was selected from the Ecoinvent 3.5 database, which consists of the recovery of the cooling utility of a cogeneration unit that uses natural gas with an absorption chiller. On the other hand, the heating source considered was the heat obtained from steam in the chemical industry. The wastewater produced within the process was considered to be treated in a generic wastewater treatment plant selected from the Ecoinvent 3.5 database.

Table 1
Aspen Plus® used operation blocks in the flowsheets for Scenarios A and B.

Common unit operation blocks

Equipment name	Aspen Plus name	Description
P-1	Pump	Pump for liquid input stream Discharge pressure 10 bar
E-1	Heater	Heat exchanger to heat liquid input stream Discharge temperature 100 °C (use of hot utility)
C-1	MCompr	Isentropic 3-stage air compressor Discharge pressure 10 bar
M-1, M-2	Mixer	Mixers
R-1	RStoic	Stoichiometric reactor Models reactions attending to specified conversion

Unit operation blocks Scenario A

Equipment name	Aspen Plus name	Description
V-1	Valve	Expansion valve Outlet pressure of 3.5 bar to perform adiabatic flash
E-2	Heater	Heat exchanger to cool reactor output stream Discharge temperature 30 °C (use of cold utility)
F-1	Flash2	Two phase flash unit operating at 1.5 bar and 30 °C
P-2	Pump	Pump for liquid stream 11 Discharge pressure 3 bar
CR-1	Crystallizer	Crystallizer Operating temperature 25 °C and pressure 2.5 bar
FI-1	Filter	Drum rotary vacuum filter Brownell filtration model
S-1	FSplit	Stream splitter to purge

Unit operation blocks Scenario B

Equipment name	Aspen Plus name	Description
F-1	Flash2	Two phase flash unit operating at 1 bar and 100 °C
F-2	Flash2	Two phase flash unit operating at 1 bar and 37.5 °C
D-1	DSTWU	Vacuum distillation unit Total condenser Reflux ratio 0.13 10 stages Operating pressure 0.55 bar
S-1, S-2	FSplit	Stream splitters to purge
F-3	Flash2	Two phase flash unit operating at 81 °C and 0.55 bar
P-2	Pump	Pump for stream 18 Discharge pressure 1 bar

2.4.3. Environmental modelling approach

The evaluation was based on the attributional LCA approach. Classification and characterization calculations were performed in the LCIA phase, but normalization and weighting results were not determined. The ReCiPe 1.1 hierarchist method [38] was implemented at the mid-point level through the SimaPro 9.0 software. In characterization, the objective is to translate quantitative inventories into environmental impacts by applying the characterization factors within the selected method. The environmental impacts of the system under study will be presented according to the following impact categories: global warming expressed in kg CO_2 eq (GW), ozone depletion in kg CFC11 eq (OD), ozone formation in kg NO_x eq (OF), terrestrial acidification in kg SO_2 eq (TA), freshwater eutrophication in kg P eq (FE), marine eutrophication in kg N eq (ME), freshwater ecotoxicity in kg 1,4-DCB eq (FET), marine ecotoxicity in kg 1,4-DCB eq (MET), human toxicity in kg 1,4-DCB eq (HT) and fossil scarcity in kg oil eq (FS). These categories

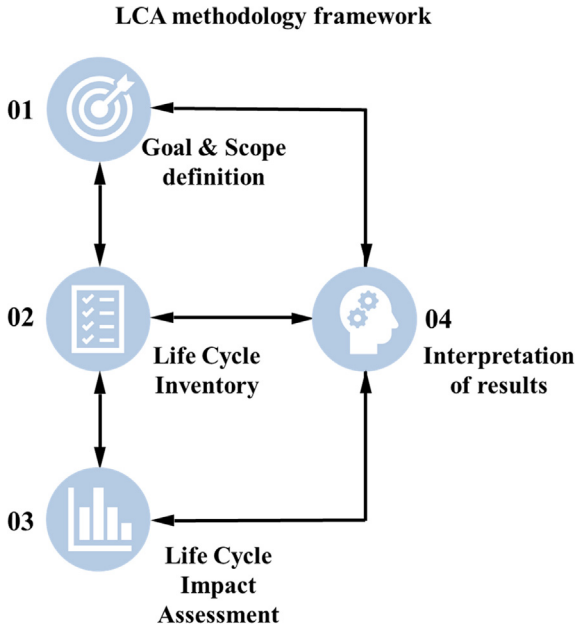

Fig. 6. Life Cycle Assessment methodology. Adapted from [29].

are considered to represent in a comprehensive way a range of potential environmental issues derived from the processes under study. Many biorefinery-related peer reviewed articles have assessed their systems considering indicators related with climate change, eutrophication, acidification, toxicity and ozone depletion/formation [9,39,40].

3. Life cycle inventory (LCI)

The detailed flow balances resulting from the simulation make up the gross inventories for the LCI phase of LCA. The simulations for Scenario A was conceived with a processing capacity of 47.5 kg/h and an output flow of 58.8 kg/h with 98% FDCA. In Scenario B, the consumption of HMF was 45.5 kg/h to produce an output of 55.7 kg/h with a purity of 99.7% Basic mass and energy flows for the environmental assessment are presented in Tables 2 and 3 for Scenarios A and B respectively. The data presented in the tables is normalized to the functional unit (1 kg/h FDCA). Electricity is expressed as electric kilowatt units (kW_e) whilst the use of heating energy and cooling utilities is represented as thermal kilowatt units (kW_{th}), which are differentiated for LCA modelling purposes.

4. Results and discussion

4.1. Simulation and sensitivity analysis results

The simulation model described in Section 2 presents the guidelines on how the simulation results were obtained. The simulation parameters were defined according to the approach followed in the environmental analysis. However, a sensitivity study was carried out to analyze whether minimization of energy requirements through optimization of a selection of relevant parameters could be effective. The sensitivity assessment focused on the downstream section of the represented process configuration. Results are presented on the analysis of the effect of the pressure in unit F-1 in Scenario A. In Scenario B the variables studied were the operating pressures of units F-1 and D-1. It is assumed that most of the differences in the process stem from the peculiarities found in the two separation sequences evaluated.

4.1.1. Aspen plus sensitivity analysis of Scenario A

The analysis of Scenario A was focused on the effect of the pressure variation in F-1 on the separation efficiency. The pressure was assessed

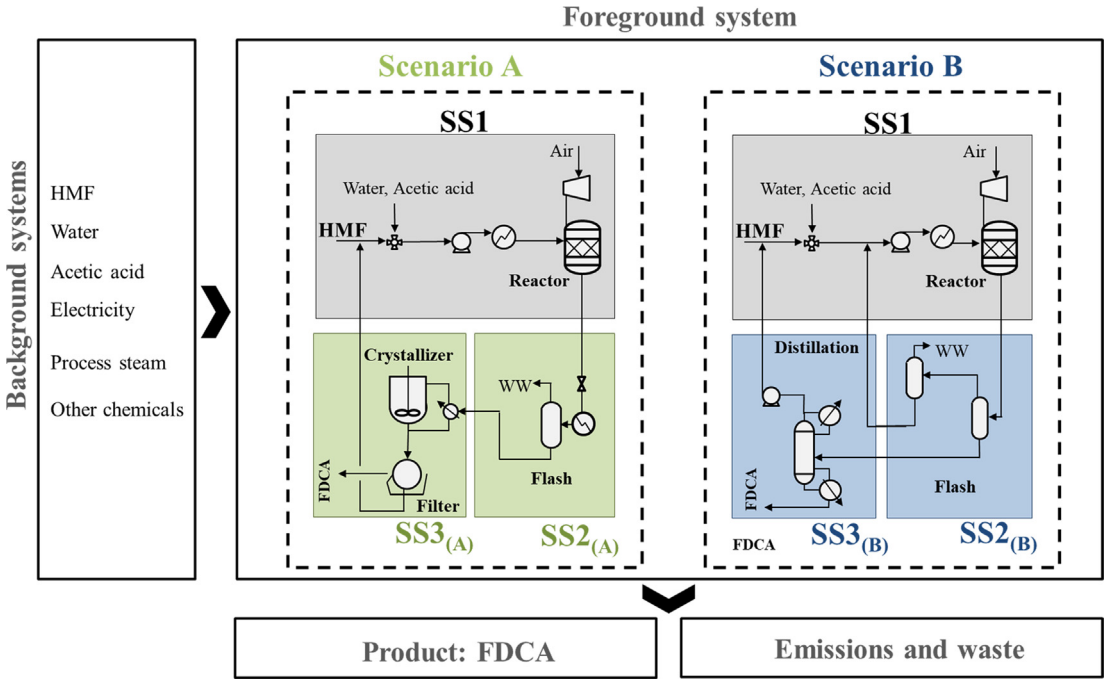

Fig. 7. System boundaries for the LCA of FDCA production considering processing units involved in Scenarios A and B (WW: wastewater).

Table 2
Life cycle inventory for the production of 1 kg/h FDCA in Scenario A (base case simulation results).

SS1. Reaction					
Input			Output		
Acetic acid	3.67	kg/h			
Water	5.50	kg/h			
HMF	0.82	kg/h			
Catalyst	0.04	kg/h			
P-1 electricity	0.02	kW_e			
E-1 heating energy	11.36	kW_{th}			
R-1 heating energy	2.72	kW_{th}			
C1-electricity	1.85	kW_e			
C-1 cooling energy	1.40	kW_{th}			
SS2. Flash separation					
Input			Output		
E-2 cooling energy	11.97	kW_{th}	*Emissions to air (vapor purge)*		
P-2 electricity	0.02	kW_e	Water	0.32	kg/h
			Acetic acid	0.23	kg/h
			Furan compounds	$5.20{\cdot}10^{-9}$	kg/h
			Nitrogen	16.62	kg/h
			Oxygen	4.64	kg/h
SS3. Crystallization					
Input			Output		
CR-1 cooling energy	3.69	kW_{th}	Wastewater to treatment	$8.90{\cdot}10^{-3}$	m^3/h

Table 3
Life cycle inventory for the production of 1 kg/h FDCA in Scenario B (base case simulation results).

SS1. Reaction					
Input			Output		
Acetic acid	3.92	kg/h			
Water	5.88	kg/h			
HMF	0.82	kg/h			
Catalyst	0.039	kg/h			
P-1 electricity	0.11	KW_e			
E-1 heating energy	8.92	kW_{th}			
R-1 cooling energy	0.51	kW_{th}			
C-1 cooling energy	1.47	kW_{th}			
C-1 electricity	1.95	kW_e			
SS2. Flash separation					
Input			Output		
F-1 heating energy	65.26	kW_{th}	*Emissions to air (vapor purge)*		
F-2 cooling energy	74.47	kW_{th}	Water	0.81	kg/h
			Acetic acid	0.33	kg/h
			Furan compounds	$9.81{\cdot}10^{-10}$	kg/h
			Nitrogen	17.57	kg/h
			Oxygen	5.02	kg/h
			Wastewater to treatment	$7.99{\cdot}10^{-3}$	m^3/h
SS3. Distillation					
Input			Output		
D-1 reboiler duty	8.24	kW_{th}	*Emissions to air (vapor purge)*		
D-1 condenser duty	8.42	kW_{th}	Water	$1.25{\cdot}10^{-2}$	kg/h
P-2 electricity	$1.14{\cdot}10^{-3}$	kW_e	Acetic acid	$8.30{\cdot}10^{-3}$	kg/h
			Furan compounds	$4.51{\cdot}10^{-8}$	kg/h
			Nitrogen	$8.86{\cdot}10^{-4}$	kg/h
			Oxygen	$2.79{\cdot}10^{-4}$	kg/h
			Wastewater to treatment	$1.12{\cdot}10^{-3}$	m^3/h

in the operation range of 0.1–1.5 bar. The sensitivity analysis of the flash unit was studied considering the resulting value of the energy demands of the equipment that can be found before or after F-1 in the production line. This was due to the fact that F-1 was simulated as an adiabatic flash with no heat duty. The effect produced was studied on the cooling required in the previous heat exchanger E-2. It was also found that the operating pressure of F-1 indirectly affected the energy consumed by the pump P-2 (Fig. 8). The needed energetic consumption

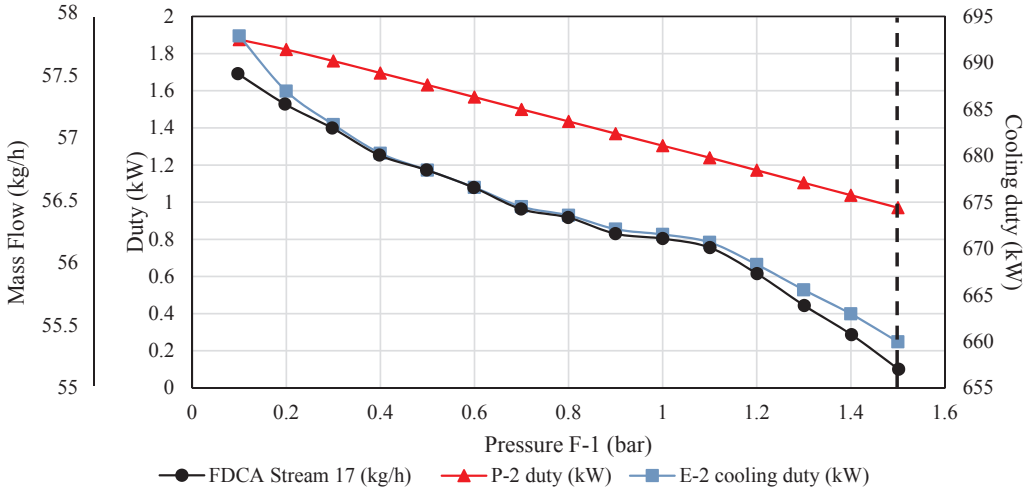

Fig. 8. Aspen Plus sensitivity analysis for Scenario A. Effect of the pressure of flash F-1 in the energy consumption of P-2 and E-2 units and the FDCA product obtained in stream 17. The dashed line represents the base case scenario conditions.

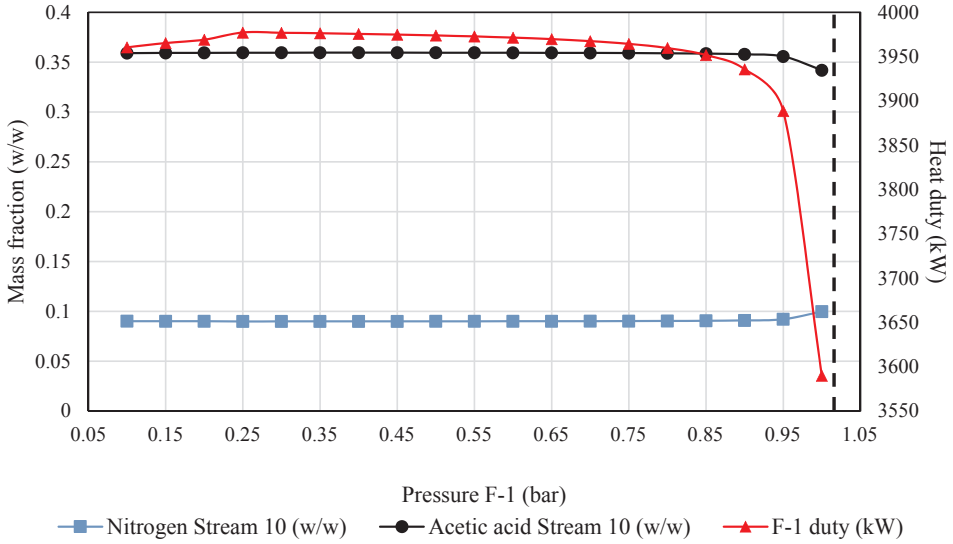

Fig. 9. Aspen Plus sensitivity analysis for Scenario B. Effect of the pressure of the F-1 flash on the mass fraction of the products present in the vapor stream (w/w) and the heating energy consumption of the unit (kW). The dashed line represents the base case scenario conditions.

that would be derived from the pressure decrease to 0.2 bar was not considered. An additional unit such a vacuum pump or an ejector would be required in that case. The mass flow of FDCA in the final output stream was also plotted to simultaneously evaluate the positive yield in the production of the main chemical and the potential decrease in the energy consumption.

It can be observed that the net energy required for the heat exchanger and the pump tend to decrease as the operation pressure of F-1 increases. The main objective of the F-1 unit is to eliminate the maximum amount of residual inert fractions, i.e. N_2, which enters the system together with O_2, for the oxidation of HMF. It can be deduced that, as the pressure of the liquid-vapor separation unit increases, the separation is improved, resulting in a reduction of the overall plant recirculating-flow. Hence, the pump P-2 and the heat exchanger E-2 require slightly lower energy consumption. Venting the spent air prior to the crystallization unit through F-1 actually ensures the correct operation of CR-1. However, the decrease of the volume in the plant has also an effect on the product flow obtained in stream 17. In general, the change of pressure in F-1 has shown that the energy consumption of E-2 could have a maximum reduction of 5%. However, the reduction in energy consumption within the operating range studied amounts to 48%. The energy consumption of P-2 is more sensitive to pressure change than the cooling needs of the previous heat exchanger. If we consider that the best Scenario for energy consumption was implemented, the FDCA mass flow would be reduced by 4% from the value corresponding to the minimum pressure considered within the range. The baseline scenario corresponds to the pressure of 1.5 bar and 30 °C, for which inventory tables have been provided.

4.1.2. Aspen Plus sensitivity analysis of Scenario B

The sensitivity analysis performed for Scenario B is based on the minimization of the energy requirements for the separation process. The two process units considered were the first separation unit, flash F-1 and the vacuum distillation column D-1.

For the pressure of the flash unit, the values of energy consumption and mass fraction of the separation were discussed. The objective of this unit is to maximize the amount of FDCA present in the output flow, as well as to simultaneously separate as much N_2 as possible leaving the column at the top. Furthermore, the separation performance in F-1 determines the extent to which recirculation of raw materials (acetic acid, water, HMF) can be achieved. For economic and environmental reasons, the overall objective of optimization objective should be to

minimize the energy consumption of the unit, provided that the operational requirements are met. The pressure in F-1 has been evaluated in the range of 0.1–1 bar. The needed energetic consumption that would be derived from the pressure decrease to vacuum values was not considered. An additional unit such a vacuum pump or an ejector would be required in that case. Fig. 9 displays the results of the first sensitivity analysis for Scenario B.

In this case, the trend for the energetic duty of the unit is to decrease as the pressure increases. Regarding nitrogen leaving the unit through the top, it tends to slightly increase as the pressure increases while acetic acid decreases. In this case, the trends of the evaluated variables behave with a somewhat stabilized response until reaching the pressure of 1 bar, at which most of the changes occur. In this unit, the optimal value of energy demand should be minimal, as expected. The nitrogen mass fraction should be maximized and, finally, the mass fraction of acetic acid in stream 10 should be minimized. The optimum operation point in this case occurs at a pressure of 1 bar (100 °C), which is again the pressure of the base case scenario considered for the simulation presented. The maximum reduction that can be achieved in the energy consumption of the F-1 flash within the temperature range studied is 9% based on the minimum pressure of 0.1 bar. A 5% reduction in the mass fraction of acetic acid can be observed in the range of pressure evaluated over the range of studied pressures. The mass fraction of nitrogen increases at a rate of 11% over the studied pressure variation.

The performance of the D-1 distillation column was analyzed by studying its operating pressure in a variable range of 0.0001–0.999 bar. On this occasion, the parameters evaluated were the heating and cooling requirements for the reboiler and column condenser respectively. In addition, the FDCA mass fraction leaving the column through the bottoms as product was represented.

The results of the sensitivity analysis are presented in Fig. 10. In this case the trends show a considerable shift of the evaluated variables in the change from 0.0001 to 0.05 bar. From 0.05 bar, the values remain somewhat constant. The direction of change in the energy consumption of the column is to decrease with increasing pressure. In other words, as pressure is lower, global net energy demand increases. However, the mass fraction of the FDCA increases as the pressure increases, reaching a maximum for pressures in the range of 0.42–0.63 bar. The increase of FDCA in the outflow presents a very slight increase (0.6%). However, the decrease in energy needs is comparatively greater, reaching 61% decrease values for both heating and cooling duties. The optimal operation would be within the aforementioned pressure range (0.42–0.63 bar), since for these values, the mass fraction of the FDCA is at its maximum, while the energy demand is within the expected reduction. The base case scenario was simulated for a column pressure of 0.55 bar, which is within the optimum range of operation.

4.2. Life Cycle Impact Assessment (LCIA)

In this section, the base case simulation results, which were presented in the inventory tables provided, are transformed into environmental impacts using the method provided in Section 2. The results in this section present the environmental profile of the two scenarios considered for the base case conditions.

First, the overall contribution to the profile of each subsystem in both scenarios has been analyzed (Fig. 11). The results are presented as relative contributions from each subsystem for Scenarios A and B. Collectively, the relative comparative loads of each scenario are represented. The figure shows, at a glance, how Scenario B has greater impacts compared to Scenario A for each impact category studied. Scenario A compared to scenario B displays 48% less environmental impacts in GW, 3% in OD, 28% in OF, 27% in TA, 46% in FE, 34% in ME, 46% in FET, 47% in MET, 32% in HT and 50% in FS. It can be observed that most of the increase in environmental impacts in Scenario B is derived from SS2. In Scenario A, SS1 is the largest contributor to impact for all impact categories. The impacts of SS2 and SS3 do not exceed 10% in most categories.

The largest contributions to SS2 in Scenario A are identified in FET, with a contribution of 14%. SS3 exhibits its highest contribution to the profile of Scenario A in the ME category, with a contribution of 4%. However, in Scenario B there is a displacement of the most burdensome subsystems within the system. The impacts of SS1 are still equivalent to the results of the scenario of crystallization. However, the burden of the SS2 experiments represents a significant increase for all impact categories compared to Scenario A. In scenario B, the relative contribution derived from SS2 acquires results with values close to 30% for the impact categories OF, TA, ME and HT and values in the 50% range for the impact categories of GW, FE, FET, MET and FS. The impact category that experiences the smallest increase in Scenario B is OD, with a contribution of 3%. This implies that stratospheric ozone depletion is not sensitive to modifications in the downstream separation process. In short, this stems from the fact that OD is a category mainly influenced by the use of DCM in this system, which is an ozone-depleting gas utilized in the upstream section of the process, for the production of HMF. Finally, in Scenario B, SS3 shows slight increases in its relative contributions with respect to Scenario A. However, these increases for all categories are not as pronounced as for SS2. In Table 4 the total contribution to impacts per category is presented for Scenarios A and B,

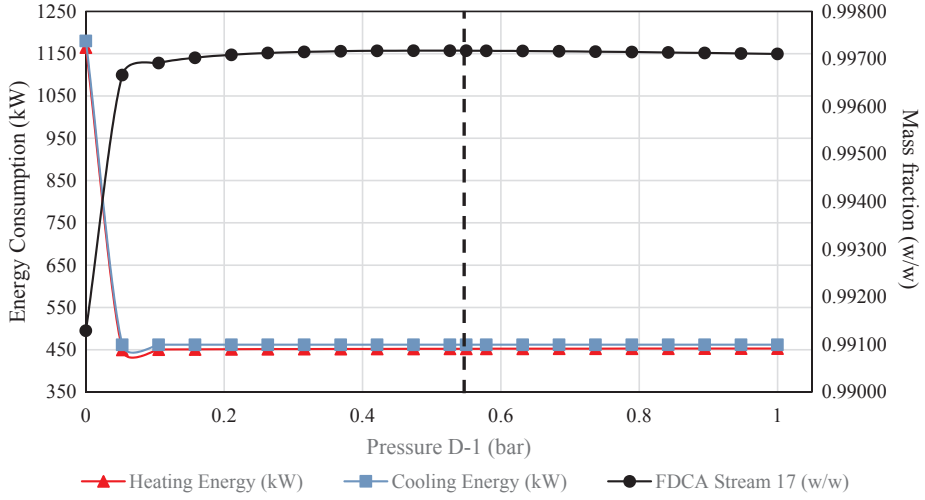

Fig. 10. Aspen Plus sensitivity analysis for Scenario B. Effect of the pressure of distillation column D-1in the purity of FDCA obtained (w/w) and the total net energy consumption of the unit (kW). The dashed line represents the base case scenario conditions.

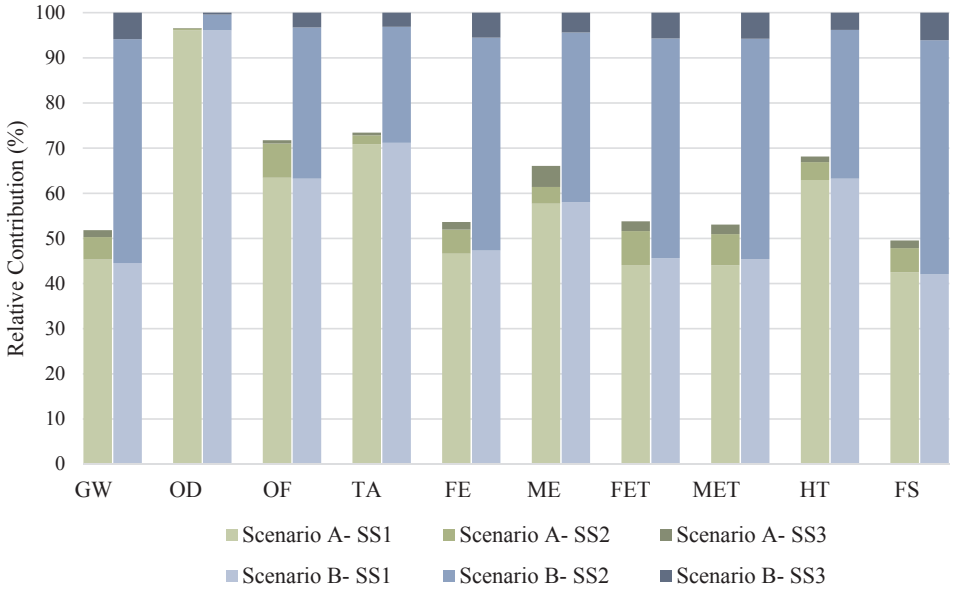

Fig. 11. Comparative environmental impacts per subsystem for Scenarios A and B considering the functional unit of 1 kg FDCA/h.

Table 4
Total environmental impacts per category for Scenarios A and B considering the functional unit of 1 kg FDCA/h.

Impact category	Units	Scenario A	Scenario B
GW	kg CO_2 eq	61.46	118.42
OD	kg CFC11 eq	4.46×10^{-4}	4.62×10^{-4}
OF	kg NOx eq	1.65×10^{-1}	2.29×10^{-1}
TA	kg SO_2 eq	2.70×10^{-1}	3.68×10^{-1}
FE	kg P eq	8.70×10^{-3}	1.62×10^{-2}
ME	kg N eq	9.56×10^{-4}	1.43×10^{-3}
FET	kg 1,4-DCB	0.82	1.55
MET	kg 1,4-DCB	1.18	2.25
HT	kg 1,4-DCB	1.75	2.57
FS	kg oil eq	18.45	37.22

with the purpose of depicting the absolute results.

It goes without saying that if any of the scenarios studied were to be improved in order to reduce their environmental impacts, the focus of the improvement work would have to be on different subsystems. In Scenario A, the revision would have to focus on SS1, while in Scenario B a reduction of impacts on SS1 or SS2 would be desirable.

To delve into the process evaluation for each scenario, their environmental profile is provided per main substance or component of their inventories. The results can be found in Fig. 12 for Scenario A and Fig. 13 for Scenario B. When analyzing the detailed results for Scenario A, it becomes clear that the greatest hotspot of the system is the production of HMF. Despite being produced from lignocellulosic biomass, its production process involves the use of organic solvents such as dichloromethane (DCM) or dimethyl sulfoxide (DMSO), which are of high environmental concern. To a greater extent, the production of HMF from lignocellulosic biomass is not yet mastered to obtain high conversion yields [32]. This is, most probably, the reason why the environmental impacts derived from a bio-based chemical show relevant contributions to the environmental profile of the system, with shares higher than 20%, reaching in multiple categories values over 60% (GW, OD, OF, TA, ME, HT and FS). DCM in the production of HMF is primarily responsible for the 98% contribution to the OD category, due to its chlorinated nature and its potential ability to impact the balance of the chemical reactions occurring in the atmosphere [41]. The use of the metal catalyst becomes apparent mainly in four categories: TA, FE, FET and MET, with impact contributions of 21, 14, 29 and 28% respectively. The impact of acetic acid is also important, although significantly lower than the impact contributions of HMF. Acetic acid has contributions above 10% most times, reaching values of 29% in some categories (FE), with the exception of OD, where a contribution of 1% is observed. The use of the cooling utility in the system has a resulting effect on most categories, also with the exception of OD. The greatest impacts of cooling energy are found in GW, FET, MET and FS. The lowest impacts on the system studied are the use of electricity, heat, wastewater treatment process and the emissions to air, which are slightly relevant in the OF category only (7%).

The profile shown in Fig. 13 presents a different scheme of the process for Scenario B. Interestingly, a rearrangement of the relative contributions can be observed again. In this case, the profile reveals that the use of cooling energy utility was the process that led to increased environmental impacts in SS2 for this scenario. There is also a smaller relevant increase in the impacts derived from the use of heat. In general, the deduction that can be drawn suggests that the substitution of the crystallization unit with a distillation column has an effect on the energy consumption of the process. Energy consumption increased by modifying the operation downstream of the process, and it was found that this increase resulted in a subsequent increase in the environmental impacts of the system. This response shows that while the energy consumption profile was not an issue in Scenario A, it became significant in Scenario B as the requirements increased. For instance, the cooling energy has a 35% contribution to the GW impact category. Cooling energy also contributes with a 38% share to the impacts in FE and with a slightly lower value to the ME category (26%). The toxicity categories analyzed have 48 and 49% contributions in FET and MET respectively deriving from the cooling utility. The contribution of this process to FS is relevant as well, representing 38% of contributions to the category. There is an apparent trend showing how the use of the cooling energy system affects the impact categories dealing with anthropogenic emissions, toxic effects on the environment and depletion of fossil resources. All these environmental effects are related to the use of a non-renewable energy source. In this study, a generic cooling energy source was selected from the Ecoinvent 3.5 database, which consists of the recovery of the cooling utility of a cogeneration unit that uses natural gas with an absorption chiller.

4.3. Environmental sensitivity assessment

The objective of the environmental sensitivity assessment is to analyze how the results of the simulation sensitivity assessment affect

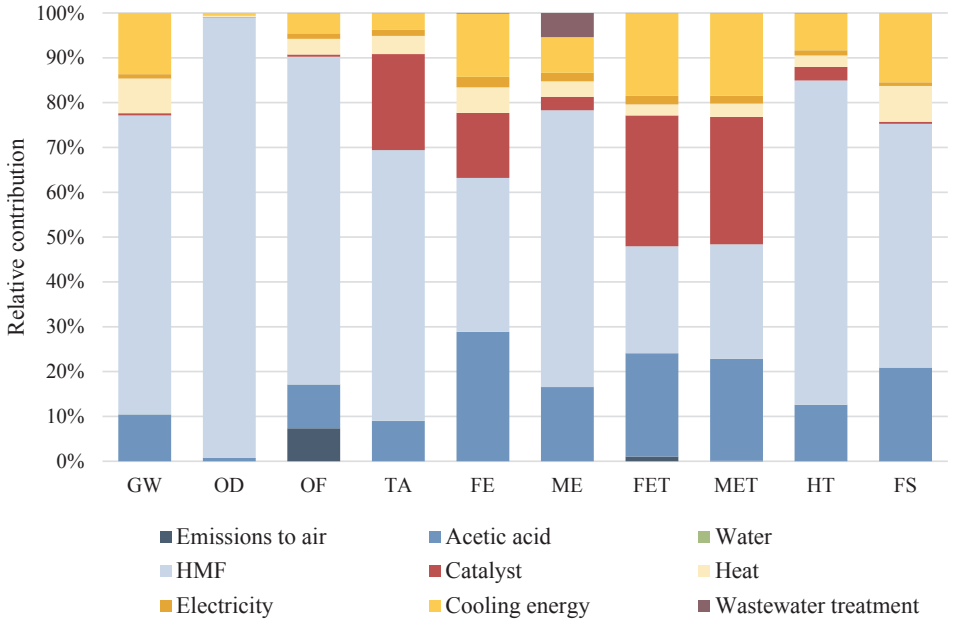

Fig. 12. Environmental profile displaying the relative contribution (%) per process for Scenario A (base case simulation results).

the environmental results obtained. In this case, not only were isolated process units analyzed, but all the simulation results of each sensitivity case study were considered to recalculate the environmental impacts of the system. The Aspen Plus simulation was computed for 3 case studies and the base case Scenario for the three variables studied in Section 3.2 (operation pressure in units F-1 for Scenario A and B and operation pressure of unit D-1 in Scenario B). The inventory tables were updated and the LCIA was conducted using the same method presented in the previous sections of this study. The results are presented in Figs. 14–16. The graphs only represent the two impact categories with the most and the least variability of their impacts to determine the overall range of variation of the environmental profile.

In Fig. 14, the objective was to analyze environmentally how the decrease in the energy requirements of the analyzed units and the consequent decrease in the product would affect the environmental results of the system. It can be observed that, as the pressure increases, the OF category experiences a quite remarkable decrease. The increase of pressure provides, as shown in Fig. 8, a decrease in the energy needed for P-2 and E-2. Furthermore, increase of pressure results in lower emissions to air and slightly lower demand for fresh acetic acid and water. These are the parameters that influence the overall increase in the impact in OF. The category among the studied that experienced the least reduction in impact was OD. In this case, the operating range in which environmental impacts would be minimized is 1.2–1.5 bar. These findings show that the environmental assessment is quite sensitive to the change in pressure of the F-1 unit for Scenario A.

Fig. 15 shows the results of the sensitivity analysis of the same unit in Scenario B. In this case, the variability of the environmental impact as a function of the pressure of the flash unit is almost negligible. The impact category that experienced the largest change was OF, with a 2%

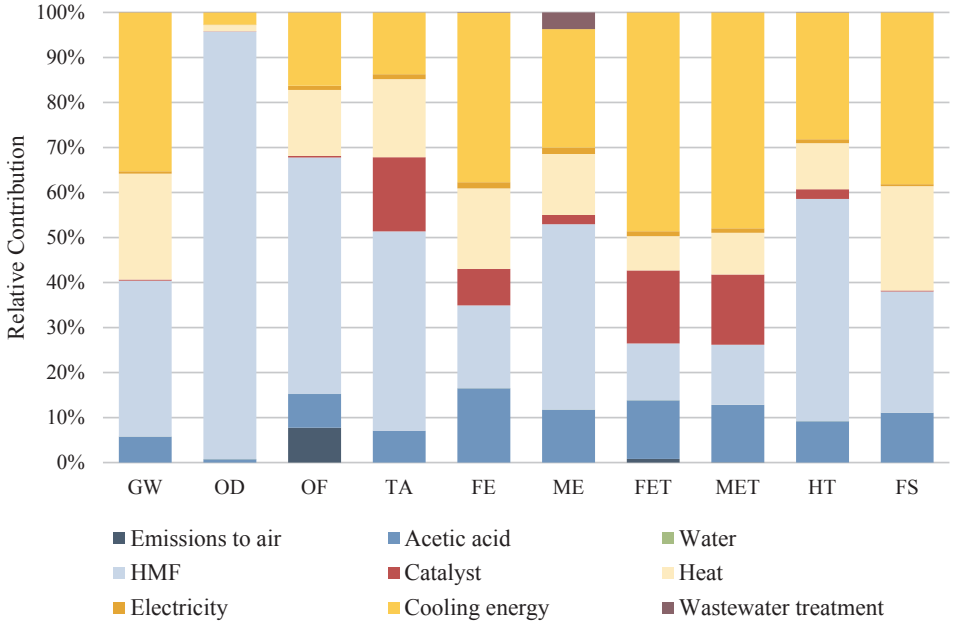

Fig. 13. Environmental profile displaying the relative contribution (%) per process for Scenario B (base case simulation results).

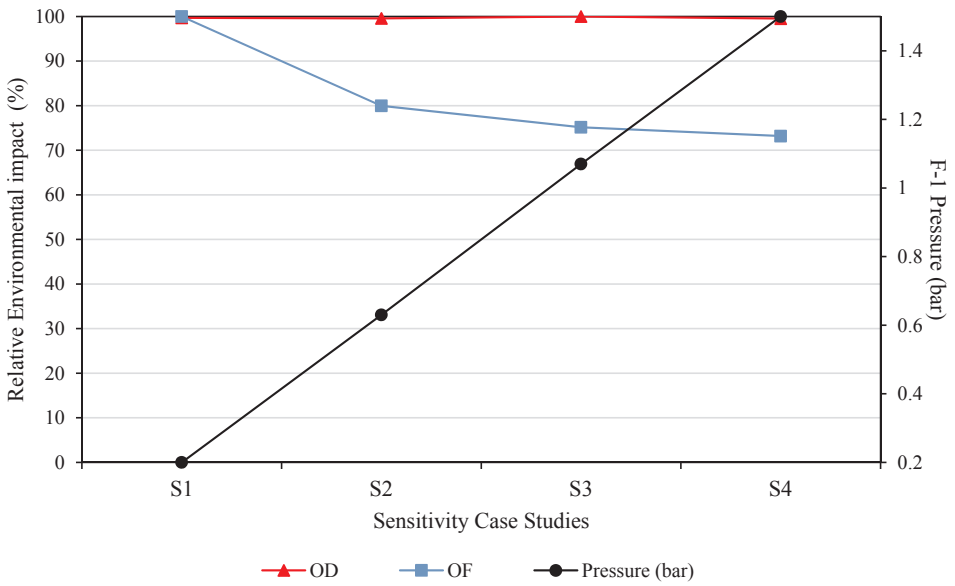

Fig. 14. Environmental results presented for OD and OF impact categories for the sensitivity study performed in the pressure of unit F-1, Scenario A. Sensitivity scenarios: S1 (0.2 bar), S2 (0.63 bar), S3 (1.07 bar) and S4 (1.5 bar).

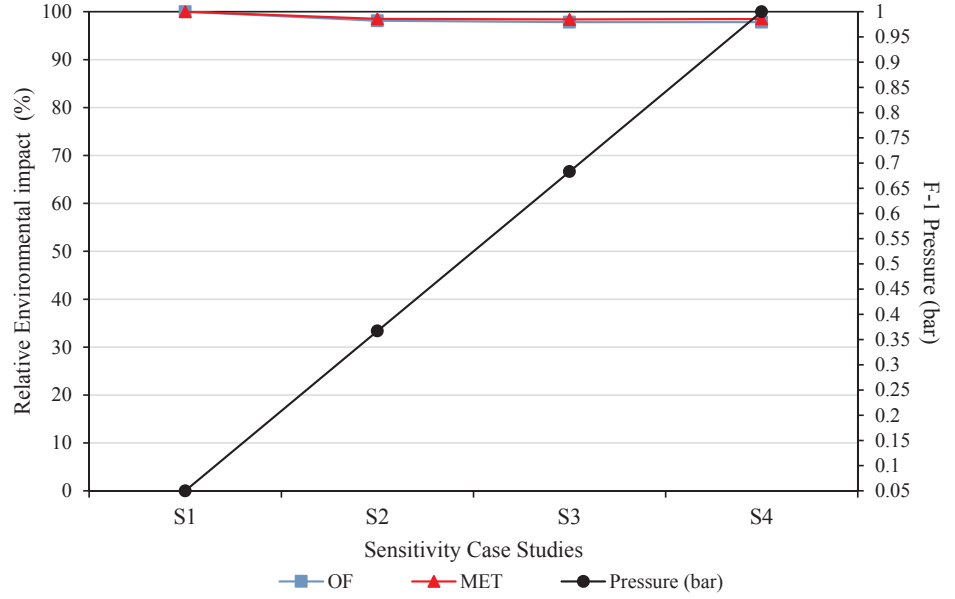

Fig. 15. Environmental results presented for OF and MET impact categories for the sensitivity study performed in the pressure of unit F-1, Scenario B. Sensitivity scenarios: S1 (0.05 bar), S2 (0.367 bar), S3 (0.683 bar) and S4 (1 bar).

improvement with increasing pressure. MET shows the lowest improvements with only a 1.5% impact reduction. In a general analysis of the scenario, the concluding observation is that the operating pressure of F-1 does not influence the overall results of the plant when analyzed from an environmental perspective.

Finally, Fig. 16 displays the results of the sensitivity assessment to the distillation unit in Scenario B. The greatest improvement in the environmental impacts was observed in FS (0.35%), while the lowest variability was that of OD (0.14%). Once again, for Scenario B, the variation in the simulated pressure for D-1 did not affect the results of the environmental assessment.

The hypothesis drawn from the results is that while in Scenario A, the effect of reduced energy consumption with decreased pressure had a reduction effect on the FDCA produced. However, in Scenario B, the increase in energy consumed was directly proportional to the production of FDCA in the system, which led to the balance of the resulting environmental impacts.

4.4. Benchmarking of LCA results for the production of FDCA

It is quite difficult to compare the results of this study with other work on the environmental assessment of the FDCA, as there are very few studies dealing with the topic. Furthermore, in studies that would somehow be under the same scope, comparability of results is very limited due to differences in the definition of the functional unit, system boundaries, method, cut-off criteria, etc.

Take, for example, the work done by Eerhart et al. [10]. Their work is based on an environmental assessment of PEF production for its comparison with PET. Therefore, their system boundaries are expanded to the polymerization of FDCA. The authors analyzed the environmental impact based on two indicators: greenhouse gas emissions (GHG) and the non-renewable energy use (NREU). Its main raw

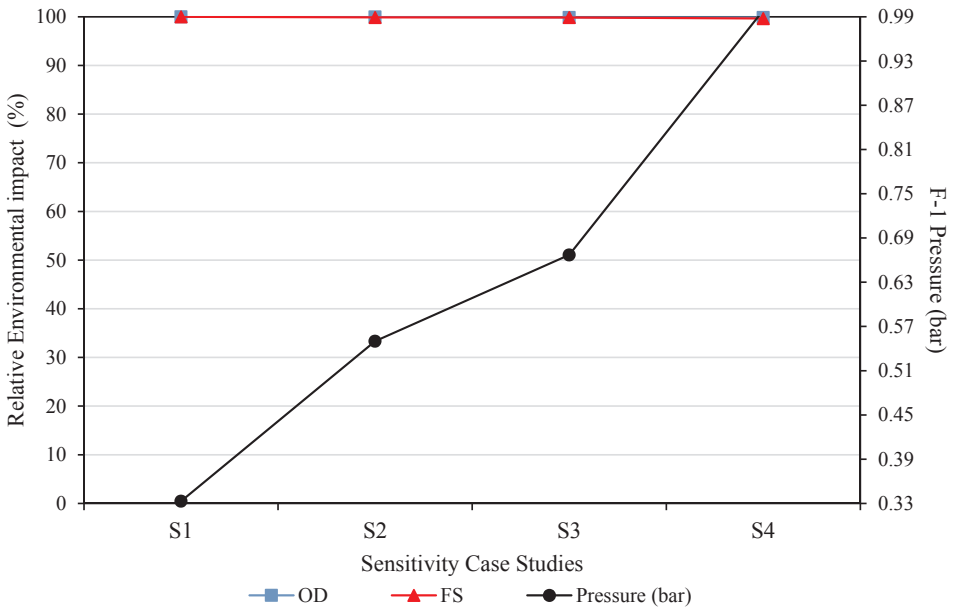

Fig. 16. Environmental results presented for OD and FS impact categories for the sensitivity study performed in the pressure of unit D-1, Scenario B. Sensitivity scenarios: S1 (0.333 bar), S2 (0.555 bar), S3 (0.667 bar) and S4 (0.999 bar).

material is fructose, which is used for the manufacture of HFM, unlike our study, which based the process on the use of HMF based on lignocellulose. Data relating to the production of FDCA by oxidation of HMF were assumed to be similar to those for the production of PTA and PET. Their system resulted in emissions of 0.59 and 0.97 kg CO_2/(kg FDCA/h) for the best- and worst-case scenarios respectively. The NREU of their study resulted in a range of 10.4–16.8 MJ/(kg FDCA/h). In our study, the GW category presented 61.5 kg CO_2 eq./(kg FDCA/h) for Scenario A and 118.4 kg CO_2 eq./(kg FDCA/h) for Scenario B. Although our results differ largely from the reported impacts in the study by Eerhart et al. [10], it is an expected behavior. Firstly, due to the differences between the boundaries of the system and the data sources of both, for example, it was mentioned above that the production of HMF was a hotspot of the system due to the immaturity of the production process. It has been reported that the production of HMF from fructose results in higher conversions [42].

On the other hand, although the authors do not mention it directly, when the GHG and NREU indicators are used, GHGs usually represent direct emissions to the environment rather than indirect emissions due to process activities. Thus, the energy use of the process could have been accounted for within the NREU indicator, drastically reducing GHG emissions. Eerhart et al. also modelled a system in which a CHP unit was used to produce energy from residual fractions of process biomass [10]. Considering that energy seems to be an important hotspot, at least on Scenario B, this can be a feasible improvement of the process to minimize overall environmental impacts.

In a more recent study [9], the authors analyzed the LCA results for the production of a polymeric material derived from FDCA. Again, their system boundaries covered the polymerization phase. HMF was considered to be obtained from fructose once again, and their inventory data was mostly retrieved from laboratory scale experiments. This implies a very different downstream separation sequence for FDCA in comparison to either Scenario A or Scenario B. Their system for the FDCA synthesis from HMF included the use of chemicals such as NaOH and $KMnO_4$. As far as separation goes, the product was filtered through a celite bed, cooled with ice and acidified with HCl. The precipitate was then vacuum pumped in a process that is the laboratory-scale variant of Scenario A, with lower yields achieved (64%).

The authors analyzed the environmental impacts as a function of GW, ecotoxicity, HT, FE, FS, TA and agricultural land occupation impact categories. Adding up the impacts of stages I, II and II of his study (corresponding to the production of fructose, HMF and FDCA), it was found that the impact for the GW category was approximately 5000 kg CO_2/kg FDCA. Their environmental impacts result in higher impacts than the results of this study. However, the comparison of results should be considered with caution, as the authors worked with assumptions different from those in the present study (e.g., transport activities were considered). In addition, the evaluation of laboratory processes through LCA has been shown to yield broader results, which are optimized as the scale of production increases [43].

Finally, in 2018, García-Gonzalez et al. [11] proposed the environmental evaluation of polyester binders containing FDCA. They studied the NREU from the Cumulative Energy Demand method [44] and the GHG through the Greenhouse Gas Protocol [45]. In this case, again GHG constituted the contributions of direct emissions into the atmosphere from fossil and biogenic sources, as well as the emissions from land use change. Total GHG emissions from FDCA production from sugar beet resulted in 1.18 kg CO_2 eq/kg FDCA, while for NREU 16 MJ/kg FDCA were reported. The results of this study are more similar to those [10], probably due to the similarity in the accounting of emissions and selected indicators.

For both Isola et al. and García-González et al. [9,11] neither inventories nor functional unit were time bound data, as it may be expected from any laboratory experimentation. Therefore, the functional units (kg FDCA rather than kg FDCA/h) make their results not 100% comparable to our study. However, it is the best possible approximation considering the fact that there are virtually no LCA studies in the production of FDCA in the literature.

The high variability of the results shows the need to develop more research on the topic, working on production routes that lead to stable and high FDCA yields and through LCA studies that present in detail their approach to evaluation for comparability reasons.

5. Conclusions

Simulation through Aspen Plus and LCA were performed for an FDCA production system. FDCA is considered a top chemical within the biomass-derived platforms and has high potential the be the building block of PEF production. The study presents how relevant separation parameters in the simulation affect the performance of the process and

the LCA results of two scenarios that are intrinsically different. In Scenario A, FDCA separation is achieved through product crystallization and filtration while in Scenario B a distillation column is used instead. LCA shows that SS1 is the most burdensome subsystem in Scenario A. In Scenario B, impacts increased due to the higher use of energy in the separation, which mainly affected SS2. HMF emerged as a relevant hot spot for both scenarios, with very relevant environmental impacts of more than 30% in most impact categories. The operating pressure in flash and distillation units for both scenarios affects plant operation by influencing total energy consumption and FDCA production. The pressure in Scenario B for F-1 and D-1 did not show a variability of the environmental results for any impact category. Based on the results obtained from this study, it would be interesting to analyze, in future research, a scenario in which most of the fossil energy sources would be replaced by renewable energy sources. For example, this could be done through the implementation of a CHP unit burning biomass residues from the process and producing energy for self-use. This study provides relevant information in the basic design phases of novel processes that can help to optimize the development of the process, not only from an economic but also from an environmental point of view.

Acknowledgments

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