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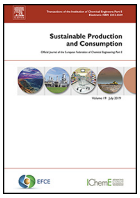

Research article

Developing future visions for bio-plastics substituting PET – A backcasting approach

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ABSTRACT

The demand for plastics far exceeds that for any other bulk material and is expected to grow further due to global economic and population growth. Packaging is by far the largest end-user segment for plastics. Interest in bioplastics is increasing as public awareness of plastic waste accumulation in natural environments increases. 2,5-Furandicarboxylic acid (FDCA) is the key monomer in the production of polyethylene 2,5-furandicarboxylate (PEF), a polymer that offers a sustainable solution to replace the commonly used polymer polyethylene terephthalate (PET). A backcasting workshop with 42 experts was held to identify current barriers and challenges that block the commercialization of FDCA-based products and to outline potential pathways toward future market diffusion. Several barriers which are strongly related to technological and market-related aspects are preventing the full potential of FDCA from being unlocked. FDCA products cited in the literature are versatile and cover a wide array of niche applications. In the backcasting workshop, participants described their specific – yet highly divergent – future visions for PEF. Participants with a background in FDCA production referred mostly to developments that would need to take place in the field of FDCA applications to turn their vision into reality, while participants with a background in FDCA product development tended to refer to open issues related to FDCA synthesis. The findings of this study indicate that there is a great need for intensified cross-disciplinary communication and collaboration.

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1. Introduction

The economic success of plastics is reflected in the enormous growth of its production in recent decades. In 1950, 2 million tons of plastic were produced worldwide; since then, the annual production has increased almost 200-fold, reaching 381 million tons in 2015 (Geyer et al., 2017). Today, the demand for plastics far exceeds that for any other bulk material (e.g. steel, aluminium, or cement) and has almost doubled since 2000 (International Energy Agency, 2018). This demand is expected to grow further due to global population growth and increasing income. According to the Ellen MacArthur Foundation (2016), almost 90% of the feedstock for these enormous production volumes is derived from fossil resources, which makes the plastic sector highly dependent on these finite raw materials. Currently, about 4-8% of the world's oil production is invested in the manufacture of plastics, with one half being used as a material feedstock, and the other half, as fuel for the production process (Ellen MacArthur Foundation, 2016). Moreover, if the strong growth trend in plastics production continues, the plastics industry could represent 20% of the total global oil consumption by 2050 (Ellen MacArthur Foundation, 2016). This development can also be attributed to the shift in the packaging sector from reusable packaging to packaging designed for immediate disposal, which is also facilitated by the inexpensive nature of these materials (Barnes et al., 2009; Jambeck et al., 2015).

Data from Geyer et al. (2017) show that the packaging market is by far the largest end-user segment, accounting for more than one-third of the demand for global plastics. This segment includes consumer packaging, such as PET beverage bottles, the packaging used in industry at large and in the business-to-business sector. In total, about 42% of all non-fibre plastics are used in this segment, which are mainly composed of PE, PP and PET (Geyer et al., 2017;

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International Energy Agency, 2018). Plastic packaging volumes are expected to continue to grow strongly, more than quadrupling to 318 million tons annually by 2050 (Ellen MacArthur Foundation, 2016).

These numbers illustrate the success of plastics, but they also provide a developmental perspective that is expected to accompany this mass production and the projected surge in consumption. Public awareness about the consumption of plastics is increasing due to an increasing awareness of waste accumulation in natural environments and the harmful effects of this plastic on wildlife that ingest or become entangled in these plastics (Thompson et al., 2009). Concerns have also been expressed about chemicals that leach from plastic products and the potential for plastics to transfer these chemicals to wildlife and humans (Ellen MacArthur Foundation, 2016; Thompson et al., 2009). In addition to these concerns, reduction of greenhouse gas emissions as a strategy to meet climate change is demanded, e.g., in several policy papers (e.g. European Green Deal). With regard to such ambitions, improvements in the field of plastics and utilised feedstock are also under discussion, since the vast majority of these are produced from fossil-based raw materials.

To address some of these issues, the increasing interest in bio-based plastics is being encouraged (RameshKumar et al., 2020) because unlike conventional fossil-resource based plastics, they are often considered to cause lower greenhouse gas (GHG) emissions (Coppola et al., 2021). Such bio-based and/or biodegradable plastics include a variety of different polymers, like naturally occurring polymers such as polyhydroxyalkanoates (PHA) or starch, but also polyesters that are obtained from bio-based monomers such as polylactic acid (PLA) (Reichert et al., 2020; Ramesh & Vinodh, 2020). Packaging applications have been the main field of interest so far, but developments in the bioplastics area are ongoing and new bio-based monomers and compounds are continually being introduced. Research on end-of-life solutions besides biodegradability, such as recycling, is also ongoing (European Bioplastics, 2015).

Polyethylene furanoate (PEF) represents one promising development in this area. This polymer is seen as an alternative to the widely used, fossil-based polymer polyethylene terephthalate (PET) due to its superior barrier properties and the fact that it can be produced from ethylene glycol and 2,5-furandicarboxylic acid (FDCA) (Coppola et al., 2021). PEF also is considered to have potential environmental advantages over PET, as it could enable a reduction in non-renewable energy demand and in GHG emissions (Eerhart et al., 2012). The first step towards implementing a PEF recycling stream was taken in 2017. This "European PET Bottle Platform" was awarded an interim approval to recycle PEF in the European bottle recycling market (BASF, 2017; EPBP, 2017) under the condition of a maximum allowed penetration of 2%.

FDCA is the key monomer in PEF production and belongs to the furan class (Sousa et al., 2016). Its structural similarity to terephthalic acid (TPA) makes it a suitable substitute for fossil-based TPA, a predominant compound in polymer and resin production, with a potential market size of several €100 M per year (Wojcieszak and Itabaiana, 2019). Moreover, for a similar role in the polyester (i.e. the rigid aromatic block), the use of FDCA instead of TPA will represent an economy of atoms – and especially carbon atoms – as TPA possesses eight carbons, while FDCA has only six (i.e. FDCA has 25% fewer carbons than TPA). Considering that, early or late, biobased or not, most carbon will end up in the atmosphere, such a reduction is environmentally relevant. This economy of atoms in the fabrication of chemical products represents one main pillar of the green chemistry principles. Therefore, the suitability of using FDCA to generate PEF has earned it the title of a “sleeping giant” (Sousa et al., 2015; Tong et al., 2010). According to Wojcieszak and Itabaiana (2019), however, FDCA is also being considered as a promising building block for a variety of other downstream products and applications. It represents a suitable monomer to produce polyesters, polyamides, polyurethanes, thermosets and plasticizers. This variety of possible materials results in a broad range of applications, for example, in plastic bottles, packaging, fibres, textiles, resins and films (Wojcieszak and Itabaiana, 2019). FDCA has been identified as a key near-market platform chemical and was already listed as one of the top twelve high-potential biobased products by the U.S. Department of Energy in 2004 (Bozell and Petersen, 2010). In 2011, the Dutch company Avantium took an important step to promote the industrialization of FDCA with a pilot plant that produced 40 tons per year (Sajid et al., 2018). This company also plans to commission a flagship plant with a production capacity of 5 kilotons per year by 2023 (Avantium, 2021a). Nevertheless, despite these advances in FDCA research and promising applications, this platform molecule still has no relevant market share (Sajid et al., 2018).

The goal of this study is to identify current barriers and challenges that block the commercialization of FDCA-based products and to outline potential pathways towards future market diffusion. In this paper, we describe possible future visions for FDCA-based products and the ways that these visions can be achieved. The following research questions were developed:

- What future visions regarding FDCA do different actors (e.g. R&D, academia, companies) in the European community (along the value chain and from lab to industry) share?
- What milestones do different actors consider as relevant to reach the respective future visions?
- Which barriers and incentives moderate the commercialization process of FDCA and related products?
- Can any differences be identified in the visions of the future between different actor groups?

2. Literature review

Several recent reviews are available on various aspects of FDCA production, such as packaging applications (Pandey et al., 2021; Sousa et al., 2021), feedstock and production approaches (Heo et al., 2021; Hwang et al., 2020), as well as life-cycle (LCA) and techno-economic (TEA) aspects (Davidson et al., 2021; Al Ghatta et al., 2021). Al Ghatta et al. (2021) simulated and compared different FDCA production options, which were evaluated on the basis of the respective MSP, carbon dioxide emissions, solvent cost, safety, and technology readiness Davidson et al. (2021). have reviewed existing TEA and LCA literature on HMF and FDCA production, providing conclusive tables on key features, and formulating valuable recommendations for future research and LCA/TEA directions.

2.1. Techno-economic assessments of PEF and FDCA

Eerhart et al. (2015) calculated the production costs of biorefinery scenarios that convert wheat straw into PEF and several co-products (capacity: 80 kt/year PEF), and found that the production of PEF was feasible at certain levels of production scale (min. 80 kt/year PEF), wheat straw cost (max. 150 USD/t), and by-products' prices. Capital costs and discount rate were identified as sensitive factors (Eerhart et al., 2015).

Regarding FDCA, several classic techno-economic assessments have been performed, calculating minimum selling prices (MSP) for FDCA by applying different scenarios and assumptions. E.g., the estimated ranges of MSPs were 1802 USD/t at a production capacity of 51,349 t/year FDCA (feedstock: high-fructose corn syrup; Dessbesell et al., 2019), 2458 USD/t (capacity: approx. 13 t/day FDCA; feedstock: HMF; Triebl et al., 2013), 1024 USD/t (capacity: approx. 296.74 t/day FDCA; feedstock: white birch; Kim et al., 2020), 2000±500 USD/t (capacity: 185 t/day; feedstock: furfural; Dubbink et al., 2021), with the market price of TPA serving as a reference in all cases.

Sensitive factors identified were, mainly but not exclusively, related to catalysts (Dessbesell et al., 2019; Triebl et al., 2013), feedstock costs (Triebl et al., 2013; Dubbink et al., 2021; Eerhart et al., 2015), FDCA selling prices (Dessbesell et al., 2019), plant capacity (Triebl et al., 2013; Eerhart et al., 2015), and total capital investment (Dessbesell et al., 2019; Kim et al., 2020; Dubbink et al., 2021; Eerhart et al., 2015).

2.2. Environmental sustainability of PEF and FDCA

Assessing the sustainability of bioplastics is not trivial, as there are several important sustainability requirements, e.g., related to the feedstock used, the production process, the use phase, and end-of-life scenarios (e.g., Álvarez-Chávez et al., 2012). As regards, for example, rthe feedstock use, the debate on food-vs.-fuel (“1st generation” food crops vs. “2nd and 3rd generation” non-edible crops, by-products, residues, and wastes) as well as crop cultivation conditions (required arable land, pesticides, fertilizers) impact the sustainability of a product (e.g., Álvarez-Chávez et al., 2012; Reichert et al., 2020). At the process level, the application of sustainable chemistry and materials development principles influences sustainability; these include, for instance, the efficient use of renewable energy, the reduction of hazardous compounds, and the generation of useful by-products (e.g., Kümmerer et al., 2020; Álvarez-Chávez et al., 2012).

While the contribution of the use phase to overall sustainability plays an important role in studies, e.g. on comparably lighter materials in automotive applications (Beigbeder et al., 2019), this particular phase is usually excluded in sustainability assessments of packaging materials, mainly because the impact of this phase is either considered insignificant or identical with the fossil-based alternative. On the other hand, end-of-life scenarios (incineration, landfill, composting, digestion, and different chemical and mechanical recycling options) play a significant role for the sustainability of bio-based plastics in packaging applications (e.g., Reichert et al., 2020). In practice, however, the end-of-life approaches are often uncertain (theory vs. practice) and vary by region (Reichert et al., 2020).

Comparing the environmental impacts of FDCA or PEF (bio-derived) and TPA or PET (fossil-based), differences are found in the respective study cases. For example, Eerhart et al. (2012) found that between 440 and 520 PJ of non-renewable energy use and 20 to 35 Mt of CO2 equivalents could be saved, if all PET bottles produced worldwide were substituted by PEF bottles (i.e., approximately 15 Mt per year). These savings would be reduced if the effects of indirect land use changes were considered, but they might also be increased if lignocellulosic biomass could be used as feedstock in the future. In contrast, Kim et al. (2020) found that fossil-depletion impacts were lower, however, climate change impacts were higher for FDCA as compared to TPA (Kim et al., 2020). Changing the underlying electricity source (from natural gas to, e.g., renewables) or using other feedstocks (e.g., corn stover or organic waste instead of white birch) would potentially contribute to a better environmental performance, according to this study (Kim et al., 2020) Bello et al. (2019., 2020) identified environmental hotspots in selected FDCA production routes: these were related to the use of HMF, energy demand (e.g., operating pressure), and solvents (e.g., DMSO and DCM). In an eco-toxicogenomic assessment of soil toxicity, results indicated that in the production chain of FDCA and TPA caused no significant gene expression changes with underlying conditions, but HMF affected several genes and processes in the model organism and could eventually be transformed into a genotoxic and mutagenic compound (Chen et al., 2016a) Maaskant and van Es (2021). investigated the UV stability of PEF in comparison to PET, and since they found that PEF showed more significant signs of degradation after UV irradiation, the authors recommended further in-depth studies on the underlying factors and mechanisms. Chemical recycling of PET in presence of PEF was reviewed, and it was found that papers and thus knowledge about chemical recycling of PEF is still limited (Siddiqui et al., 2021).

3. Methods

3.1. Backcasting

Robinson et al. (2011) defined the application of the backcasting approach in futures studies as ‘the articulation of desired futures, and the analysis of how they might be achieved’. This definition was used as the guiding principle in the backcasting approach chosen in this study. The method was implemented in an online workshop with 42 researchers and industry representatives who participated in the FUR4Sustain COST Action (https://fur4sustain.eu/) in Fall 2020. The participants origin from 15 different European countries with most being affiliated to universities, but also research centres and companies.

Backcasting was developed in the energy sector, where it was first introduced as an alternative method for planning the supply and demand of electricity (Lovins, 1976). The predominant forecasting methods used at the time were applied to make predictions about the future based on current observations, whereas backcasting begins with a predefined future and ways to achieve this future are subsequently derived (Grêt-Regamey and Brunner, 2011). According to Robinson et al. (2011), the approach has been expanded to include a more general method of analysing alternative desired futures, and particularly those that address sustainability issues and can be applied at national and local scales. In addition, the backcasting approach can be taken to shift the focus away from scenarios created by researchers to achieve externally defined goals and toward participatory approaches, considering the preferred futures of stakeholders (Robinson et al., 2011). According to Quist and Vergragt (2006), the participatory nature of backcasting analyses implies that researchers can more directly examine the complex processes required for sustainable developments and changes in current production and consumption systems. Due to the inherent uncertainty of the future and the ambiguity of stakeholders with their different value sets and mental frames, industrial transformations are processes that involve technological, cultural, social, institutional and organizational changes. Such changes also affect many stakeholders when they diffuse into society and can involve complex processes of social change over the long term (Quist and Vergragt, 2006).

To incorporate the backcasting approach into a time-limited, online workshop, the methodological framework as described in Quist and Vergragt (2006) and applied by Partidario and Vergragt (2002) was adapted to this setting. In order to maintain the crucial participatory, interactive element of backcasting in this situation, the interactive presentation software Mentimeter was chosen. Mentimeter is a tool that can be used to create presentations that allow audience engagement in an online setting. The interactive element consists of questions and polls that can be answered in real time during the presentation by the participants via their own smartphones or computers (Mentimeter, 2021). The biggest advantage of using this tool as compared to traditional survey or interview methods is that it increases the contextual relevance for each participant, since it is carried out in a mutually attended workshop, and all answers are immediately visible in the presentation. This, in turn, can stimulate new thought processes and in-

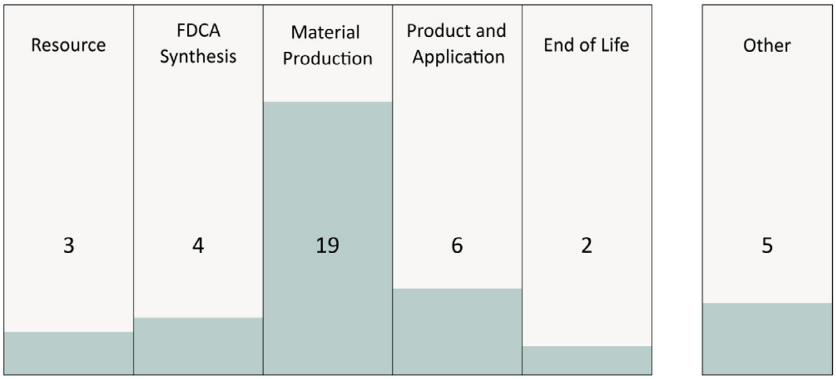

Fig. 1. Assignment of workshop participants according to their professional backgrounds (n = 39).

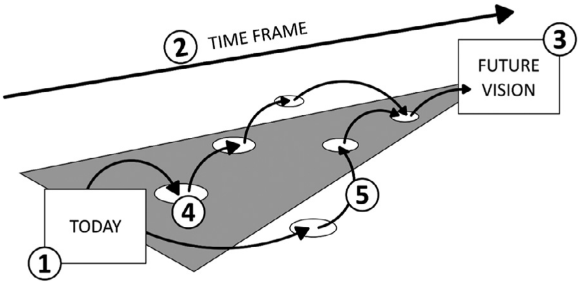

Fig. 2. Illustration of the backcasting process applied in the stakeholder workshop (adapted from Grêt-Regamey and Brunner, 2011).

crease social learning among participants, which takes full advantage of the inherent value of participatory processes as tools for social change (Robinson et al., 2011).

In a first step, the value chain of FDCA and the respective affiliations of the participants to particular elements of this chain were considered. Therefore, at the beginning of the workshop, the participants were asked to indicate their affiliations to elements in an illustrated value chain of FDCA products, according to their professional backgrounds (Fig. 1).

The next steps in the workshop were carried out by following the scheme suggested by Grêt-Regamey and Brunner (2011), as shown in Fig. 2. First, the current sustainability and market-related situation of FDCA-based products was summarized on the basis of the results of the systematic literature review (see Section 3.2). For this purpose, ten general statements were derived on potentials, challenges and sustainability aspects related to FDCA. These statements were presented to the workshop participants, who were asked to express the level of their agreement or disagreement with the respective statements.

After the participants' levels of dis-/agreement with the general statements about FDCA were assessed, the participants were given the opportunity to supply open-ended responses to address aspects that had not been covered in the general statements, but were necessary to describe the current situation of FDCA-based products (item 1 in Fig. 2). The results of this first step could be seen by all participants. If new ideas arose as a result, the workshop coordinators pointed out that participants had the possibility to submit several answers.

The second step taken was to define the time frame for the future vision (item 2 in Fig. 2). For this purpose, the time frame was set from 2023, which is the end of the COST Action, to 2060, and participants were asked to set their target year with respect to the subsequent definition of the desired future. The mean value was calculated from all the answers given and defined as the collective target date for achieving the desired future visions.

The third step was to define the future vision for FDCA-based products (item 3 in Fig. 2). The participants were asked to consider their personal visions, regardless of the current challenges related to this topic. The collected answers were again shown to all participants, and multiple answers per person were allowed. The last two steps were carried out to find ways to connect the current situation with the desired visions of the future. First, participants were asked to define milestones that needed to be reached to achieve the desired future vision (item 4 in Fig. 2). Next, appropriate measures were defined to achieve these milestones and, finally, to achieve the desired vision for the future (item 5 in Fig. 2). The workshop participants' responses were thematically categorized to present the results in more detail.

Pearson's chi-squared test was performed in RStudio using the packages *gmodels* and *effsize.* The independence of the variables (field of employment: two categories; future vision: three categories was tested with $\alpha = 0.05$ (total observations: 58).

3.2. Derivation of statements from literature

Since a systematic review of barriers and challenges that block the commercialization of FDCA was lacking before, it was carried out in the course of this work in order to serve as a starting point for the workshop The results of the review summarize the current state of the art regarding FDCA production and processing, with a focus on market and environmental sustainability aspects. This provided a reference point in that it enabled us to identify published visions, expectations, and general statements and subsequently use these in the stakeholder workshop.

In the first step, a defined body of the literature was defined. Search terms were carefully chosen to compile a collection of literature on FDCA with a specific focus on economic or sustainability issues in order to cover market-related aspects. For this purpose, the following search terms were used to search the multidisciplinary database Scopus (search query on 27 April 2020). These terms were chosen based on the search terms used by Wenger et al. (2020), who conducted a similar literature review on lignin:

TITLE ("2,5-furandicarboxylic acid“ OR "furan-2,5-dicarboxylic acid" OR "2,5-furan-dicarboxylic acid" OR "2,5-dicarboxy furan" OR "fdca" OR "dehydromucic acid") AND TITLE-ABS-KEY ("sustainab*" OR "application" OR "market" OR "economic*" OR "financ*" OR "techno-economic" OR "value-add*" OR "value add*" OR "added value" OR "cost" OR "price" OR "money" OR "innov*" OR "valori*" OR "decision" OR "business" OR "revenue" OR "environment*" OR "green" OR "social" OR "life-cycle" OR "life cycle" OR "LCA")

The time frame for the articles and reviews was limited to the period of 2015 to 2020, although papers from an earlier period

Table 1
List of key words used to screen the selected literature.

Target issue	Search term
Economic aspects, market related aspects	value, billion, market, demand, cost, price, econom*, commercial, industr*, cheap, expensive, innov*, financ*, applic*, business, scale
Sustainability aspects	environment*, sustainab*, green, degrad*, fossil, bio*, recycl*, eco, petro*, renewable, reus*, energy
Challenges and opportunities in general	Benefi*, advantag*, potential, challenge, opportunit*, better, success, promising, important, platform, key, driver, barrier, alternative, replac*

were also considered if they were found to be particularly relevant, e.g. described visions and expectations of the FDCA development. The resulting collection of articles was examined to determine the distribution of topics covered, resources used, products manufactured and key drivers and barriers with respect to the market situation for FDCA-based products. To this end, a list of keywords was compiled to capture as many aspects of economic and environmental sustainability as possible (see Table 1).

The data extracted from the literature were sorted and processed using Excel. Recurring statements found using search terms shown in Table 1 were collected (see supplementary materials).

4. Results

4.1. Summarizing the State of FDCA Based on Literature

4.1.1. Research fields and approaches on FDCA identified in the scientific literature

By far the largest part of the literature collection ($n = 100$) consisted of papers with a technological focus, i.e. on the synthesis of FDCA from various feedstocks and/or from different roots or the production of products from FDCA (66 papers). A smaller share of the literature consists of review papers (16), while a similar number of papers (12) have a biotechnological focus, presenting investigations on the enzymatic production of FDCA or products from FDCA. A small number of papers (4) deal explicitly with environmental issues in relation to the production of FDCA. In addition, only two (2) papers were found that address techno-economic issues in relation to FDCA production.

A closer examination of the technological, biotechnological, techno-economic and environmental papers (84 in total) revealed an imbalance in the numbers of the published papers when assigned to their respective positions along the value chain. The majority of the literature collection clearly addresses the production of FDCA from various resources, with 61 papers. In comparison, only 23 papers have been published on the synthesis of products from FDCA.

4.1.2. FDCA-derived products and applications covered in the scientific literature

An examination of the applications for FDCA mentioned in the literature shows that the possibility of replacing TPA and producing PEF is consistently mentioned as a specific potential application (i.e. in 76 out of 84 papers). In addition, more general applications of FDCA in the production of polymers, mainly polyesters, but also polyamides and bio-based epoxy resins, as well as fine chemicals, pharmaceuticals and agrochemicals (e.g. Ardemani et al., 2015) are mentioned throughout the literature.

Fig. 3 shows products and applications that are covered in the respective 23 papers. We can see that only two papers deal with the production of PEF, while the remaining 21 describe a diversity of other products.

After screening the selected literature, statements S01-S10 (see Table 2) were formulated to reflect the general scientific consensus regarding the current situation of FDCA. The compact formulation was chosen to facilitate the presentation of the statements in the backcasting workshop.

4.2. Current state of FDCA based on stakeholder views

The levels of agreement with the statements S01-S10 were consistently high (see Fig. 4), with a median score of four (3) for

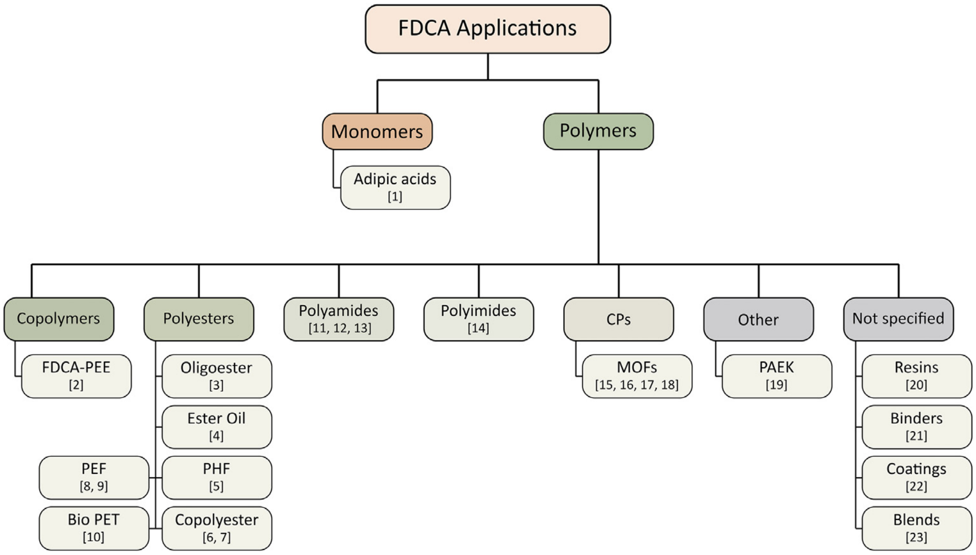

Fig. 3. FDCA products and applications identified in the literature (1 = Wei et al. (2019), 2 = Sousa et al. (2016), 3 = Cruz-Izquierdo et al. (2015), 4 = Fan et al. (2020), 5 = Zhang et al. (2019), 6 = Guidotti et al. (2019), 7 = Sun et al. (2018), 8 = Banella et al. (2019), 9 = Joshi et al. (2018), 10 = Ogunjobi et al. (2019), 11 = Cao et al. (2017), 12 = Jiang et al. (2015), 13 = Smirnova et al. (2020), 14 = Ma et al. (2018), 15 = Dreischarf et al. (2017), 16 = Ma et al. (2016), 17 = You et al. (2020), 18 = Zhao et al. (2017), 19 = Bao et al. (2019), 20 = Miao et al. (2017), 21 = García González et al. (2018), 22 = Lomelí-Rodríguez et al. (2018), 23 = Poulopoulou et al. (2020)).

Table 2
General statements about the potential, challenges and sustainability aspects of FDCA-based products.

Category	Nr.	Statement	Reference
Potential of FDCA products	S01	FDCA is a product with a high added value. There is a great potential in the utilization of FDCA.	FDCA is ranked under the top 12 biobased compounds carrying a high market potential by the U.S. Department of Energy (Bozell and Petersen, 2010; Chen et al., 2016a) and it has been considered a 'sleeping giant' due to its applications in diverse areas (Sousa et al., 2015; Tong et al., 2010).
	S02	Currently, the market for FDCA is limited.	FDCA production today is limited and only a few companies are involved in its manufacture (Bello et al., 2019).
	S03	FDCA is a promising chemical and can be an alternative to other materials.	FDCA can replace terephthalic acid, which is an important monomer to produce PET (Chen et al., 2017).
	S04	There are bright market prospects and an increasing demand for PEF.	Ban et al., 2019
Challenges in the production of FDCA and FDCA products	S05	There are still some difficulties in the production of FDCA from biomass.	There remains a challenge for researchers to develop a scalable process for synthesis of FDCA (Rathod and Jadhav, 2018).
	S06	HMF is at the moment the primary starting material for the production of FDCA.	Most efforts are directed towards FDCA production from HMF (Bello et al., 2019).
	S07	It's a technical challenge to further process FDCA into value-added products.	Factors in chemical synthesis could complicate the manufacture of products (e.g. viscosity; see Bao et al., 2019) or the products could exhibit unfavourable properties (e.g. yellow, brownish colour; see Banella et al., 2019).
Sustainability aspects of FDCA products	S08	Environmental concerns related to mineral oil are a major driver for the interest in producing FDCA from biomass.	Biomass conversion to value-added chemicals as candidates to petrochemicals has drawn tremendous attention to reduce the depletion of fossil resources (Chen et al., 2017); concerns about petroleum shortages, and environmental impacts of plastic waste production have motivated research on green alternatives to PET (Dessbesell et al., 2019).
	S09	FDCA is a sustainable, environmentally friendly product.	FDCA is presumed as a green replacement for (fossil-based) terephthalate (e.g. Wojcieszak and Itabaiana, 2019)
	S10	FDCA has the potential to reduce the dependence on fossil fuels.	FDCA is regarded as an attractive biorefinery product that could significantly reduce the dependence on fossil fuels and contribute to environmental protection (e.g. Gao et al., 2019)

statements S01-S03, S05, S06, and S08-S10. Only statements S04 and S07 resulted in a median score of three (3), which indicates a rather neutral sentiment.

Overall, this means that the workshop participants consider FDCA to be a product with a high added value and with a great potential in terms of its utilization (S01). Although the market for FDCA is currently seen as limited (S02), this molecule is considered to be a promising material that can be used as an alternative to other materials (S03). Currently, some difficulties in producing FDCA from biomass (S05) still exist, and the primary starting material is HMF (S06). FDCA was viewed by the workshop participants as a sustainable and environmentally friendly product (S09), with environmental concerns related to mineral oil use being a primary reason for the interest in producing FDCA from biomass (S08). FDCA is also considered to have the potential to reduce the dependence on fossil fuels (S10). An average level of agreement was seen with the statement that the demand for PEF is increasing and that bright market prospects, therefore, can be expected (S04). In addition, the technical barriers to the manufacture of products from FDCA were not considered to be particularly high (S07).

The next set of questions directed the attention of the workshop participants to the **economics**, and in particular the price, of FDCA, which were seen as the biggest obstacles to market introduction (Fig. 5, blue bar). The participants emphasized the facts that FDCA is currently not yet competitive with respect to oil prices and that FDCA is only available in limited quantities.

Some factors were also mentioned regarding **environmental sustainability** (green bar). All statements in this area are related to the end of life of FDCA products, such as their biodegradability, and to difficulties faced when attempted to process FDCA products together with already established materials in the existing recycling stream.

In addition, the participants pointed out important fields that do not seem to be the focus of attention so far (**'Blind spots'** – brown bar). For example, participants mentioned that the emphasis on FDCA alone is too strong and that it would make sense to investigate other FDCA derivatives and furans as well. Similarly, the strong focus on PEF as an end-use application was also critically questioned; participants pointed out that suitable niche applications for FDCA also need to be explored.

Some answers given also referred to **production and technology**. Regarding the production of FDCA, participants mentioned mainly issues associated with by-products from the synthesis and the purity of the final product, but also the thermal stability of furans, as relevant aspects (Fig. 5, grey bar). The advantages of FDCA over TPA were also highlighted based on the favourable atom economy of FDCA, and the compatibility with PET infrastructures was pointed out.

Only a few responses were categorized under **Society and Politics**; thus, these seem to be less relevant in the current situation from the viewpoint of the participants (orange bar). These answers were mainly related to the need for a shift in thinking in general. This shift would need to occur, on the one hand, in consumers regarding their acceptance of the products on the market, but, on the other hand, also in politicians who set the regulatory framework.

4.3. Visions for a future with FDCA-based products

The mean time frame for a FDCA vision was calculated from all the answers, resulting in a target date of 2033. Fig. 6 shows that participants' responses regarding their desired future vision relate strongly to **applications** for FDCA (yellow bar). In general, most statements were related to PEF. Participants described the vision that PEF would be commercially available in 2033 and mentioned different market shares. For example, completely replacing

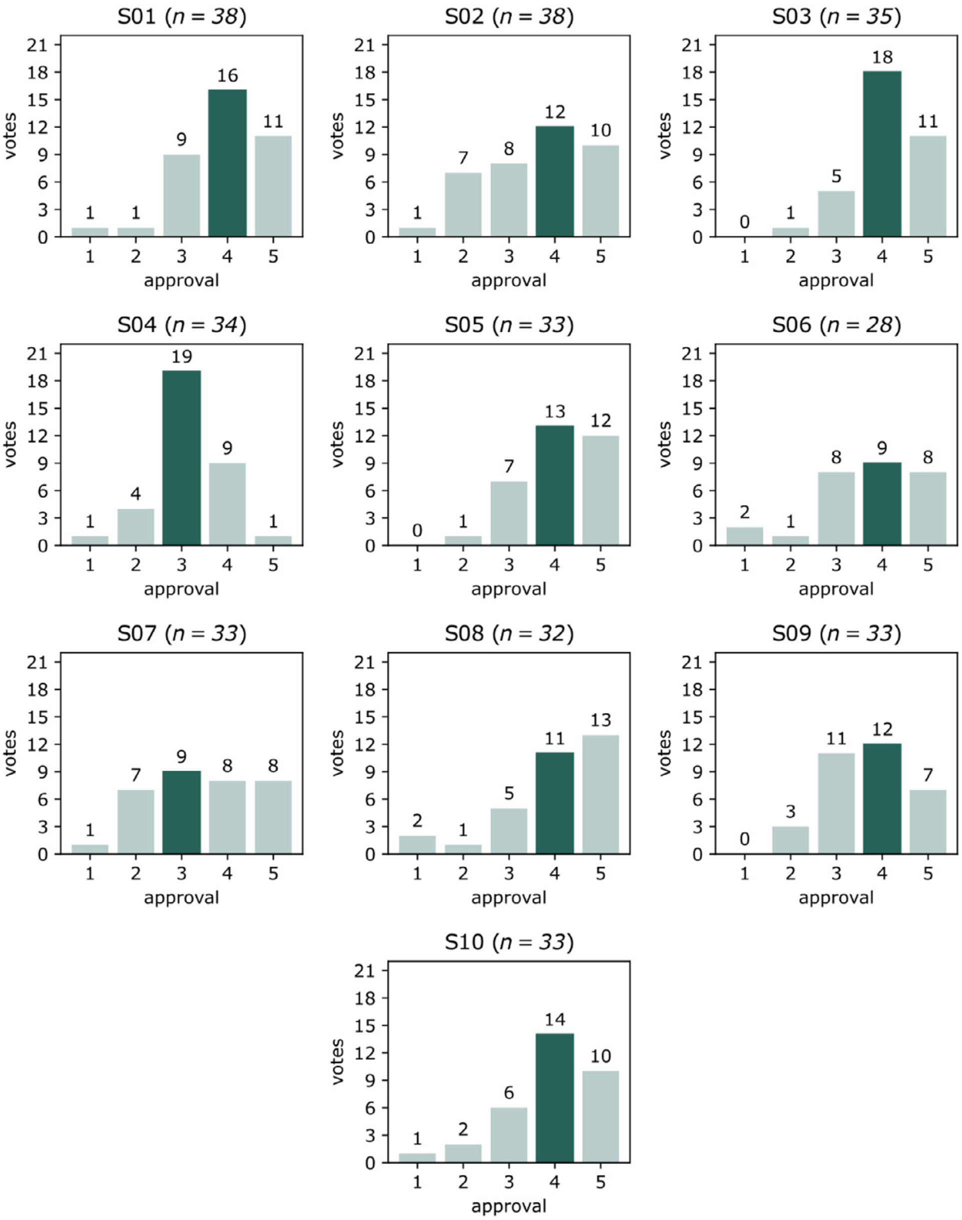

Fig. 4. Workshop participants' responses to presented statements on the current situation regarding FDCA. The level of agreement is shown on the *x*-axis (1 = strongly disagree, 2 = disagree, 3 = neutral, 4 = agree, 5 = strongly agree), the number of participants showing the respective level of agreement is shown on the *y*-axis. The dark green bar indicates the median.

TPA by FDCA or only partially replacing it (i.e. by 20–50%) was considered desirable by the different participants. Again, some participants pointed out possible applications other than bottles and food packaging for FDCA products, such as bio-based plastics used in high-performance engineering, textile fibres made of 100% PEF, or a FDCA share of 10% in polymers for coating. Moreover, in the future, FDCA-based materials could just be one of many other materials, which might only be used where needed.

Environmental sustainability also plays a prominent role in the participants' future visions of FDCA (Fig. 6, green bar). For example, a general decrease in consumption per capita was mentioned as an important aspect of the future vision. Moreover, participants predicted that recycling would be subjected to a change process, with the technical feasibility and sustainable end-of-life scenarios for FDCA products being mentioned as valid considerations.

Furthermore, some answers were given that had a stronger **economic focus** (blue bar). For example, the vision of a circular economy was expressed in which FDCA plays an important role, and a higher bio-based share is generally found in commercial products. A more economical production of FDCA products was defined as a clear target vision, for example, by increasing the availability of cheaper feedstocks and scale-up options. In addition, in the desired future vision, participants indicated that FDCA should be available at a reasonable price in conformity with the market, and thus also achieve a certain market share. In one vision, by the end of the time frame, several facilities in Europe would be able to produce FDCA for different applications and it would be able to replace its fossil counterpart if the final product is more sustainable. A global production of FDCA of 200 kt per year, of which 100 kt would be used for PEF and the rest for other applications, was also defined as a clear vision.

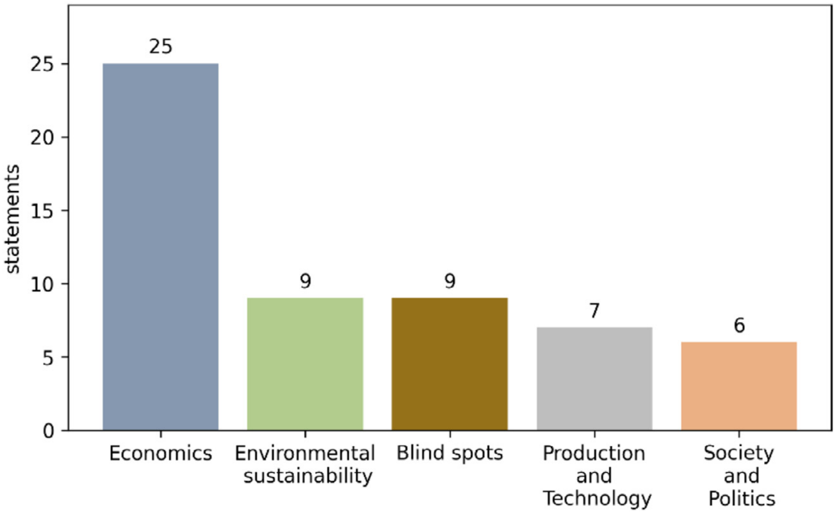

Fig. 5. Responses to challenges and opportunities with regard to FDCA products, according to thematic clusters represented by the bars ($n = 30$ participants).

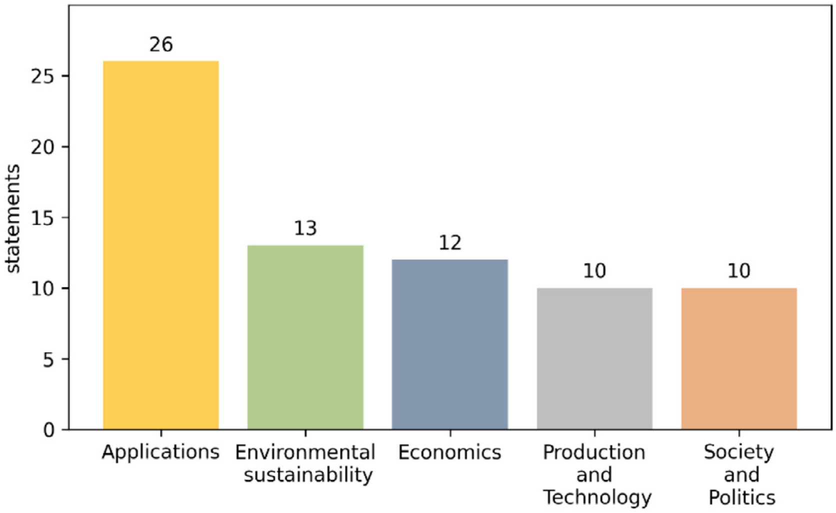

Fig. 6. Responses to the question about the idea of an ideal future vision, according to thematic clusters represented by the bars ($n = 26$ participants).

Some relevant aspects regarding **production and technology** were also mentioned (grey bar). The vision that the principles of green chemistry should also be applied in furan development, rather than placing a focus only on "green" materials, was clearly expressed. In general, improvements in furan product development were mentioned as important components of the future vision, together with the creation of further pilot and demonstration plants and additional funding for further research and process optimization. Furthermore, the production of FDCA from non-food resources was mentioned as an important component of the desired situation in the future.

In the vision of the future, as well as in the present, the roles played by **society and politics** seem to appear on the side lines (orange bar). Still, some important aspects were mentioned by the participants that are part of the desired vision of the future. These include the consumer side, where a significant amount of education and awareness about sustainable materials has happened, and the policy side, which is concerned with regulation. These aspects could be more clearly considered in the future by taking a joint approach at the European level and by promoting the production of FDCA-based products, for example, through the financing of sustainable materials and carbon taxes.

While individuals engaged in synthesis and material production in the field of FDCA referred in their future vision mainly to the market applications of FDCA, individuals engaged in the development of FDCA products and applications referred in their future visions mainly to developments in production, technology, research and development, as well as increased environmental friendliness ($p = 0.045$). The categories of economics, society and politics were named with equal frequency in the visions of the future of both professional groups (contingency table with test statistics is given in the supplementary material).

4.4. Pathways leading toward a future with FDCA-based products

In correspondence with the participants' descriptions of the present situation, the primary obstacles mentioned to achieving the desired future vision with FDCA were related to **economics** (Fig. 7, blue bar). In this context, the availability of FDCA on a larger scale and at a competitive price (e.g. less than €10/kg) was mentioned as the most important factor, but participants also mentioned the need for feedstocks to be available at low cost and a clear scale-up in production to be possible. This discussion also included the need to increase the number of FDCA producers in

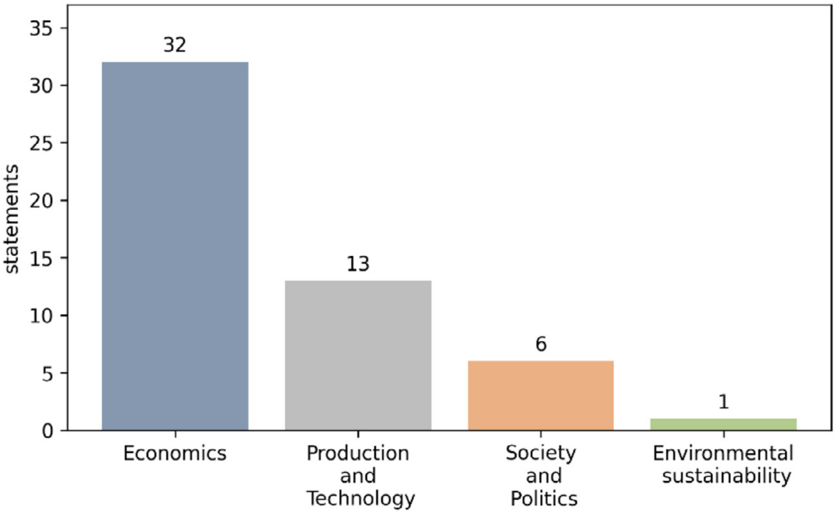

Fig. 7. Responses to the question about the milestones to be reached until the future vision is achieved, according to thematic clusters represented by the bars ($n = 22$ participants).

general and the role of investments from the European Union in order to establish larger FDCA production facilities.

Again, participants recognized replacing TPA by FDCA as another important milestone, but also saw the need to further diversify the product portfolio of FDCA.

Milestones in the area of **production and technology** represented the second largest pillar for achieving the vision of the future (Fig. 7, grey bar). Here, the participants primarily mentioned aspects such as purity or meeting technical standards of products, but also further process development. On the one hand, participants mentioned the need to achieve a fully developed sugar to furan technology, but also the need to utilize lignocellulosic biomass for FDCA production. As a further important component of these milestones, the participants saw a need for a shift in the field of research away from purely academic work and towards more applied research that involved industry, manufacturers and end users.

Again, some of the answers referred to the role of **society and politics** (orange bar). Still, the participants saw regulations (e.g. plastic bans) as important milestones in this area to promote bio-based products. The role of society was also considered as important in the sense that public opinion could influence political decisions.

Finally, one participant also mentioned the fact that furan can be regarded as safe in terms of exposure and decomposition and therefore contributing to environmental sustainability.

In the last part of the workshop, the participants were asked to describe measures that would be suitable to reach the milestones previously mentioned and to gradually achieve the vision of the future (Fig. 8). Compared to the results reported in the previous section, a shift is evident here, as participants considered the role of **society and politics** as the most important component in this part of the workshop (orange bar). Many participants emphasized their belief that a change in the behaviour of society in general will be necessary to achieve the future vision. They indicated that this change could be achieved, for example, by providing more education and information. On the political side, legislation was seen as an important tool for achieving the milestones, as it could increase investment in furan production and financial resources for further research on FDCA and FDCA derivatives. Consumers were also considered to play an important role and, above all, their willingness to pay more for bio-based products was emphasized.

Many of the proposed measures were assigned to the area of **production and technology** (grey bar). In particular, participants highlighted the need to explore alternative production methods for FDCA products, and especially methods using enzymatic routes and biotechnology. In general, they believed that sugar to furan technology needed to be improved, with several producers engaged in dedicated research. In this context, they also emphasized the need to achieve a better mutual understanding regarding the respective work being carried out by people in different professions involved in furan product research. One participant pointed out that compounding and microstructure are essential in materials processing, and awareness of this is needed among FDCA manufacturers. Finally, one participant mentioned climate change mitigation measures which were allocated to environmental sustainability.

5. Discussion

Dividing the identified literature into two categories, namely, into FDCA production and FDCA-based products categories, and comparing how many papers could be assigned to each category, papers on the synthesis of FDCA clearly dominate, while fewer papers are available on the development of possible applications of the substance. One possible explanation for this finding could be simply that a greater need for research on FDCA synthesis exists. This conclusion is also consistent with the outcome of the workshop, whereby participants strongly agreed with the statement ‘There are still some difficulties in the production of FDCA from biomass’ (S05), while they responded neutrally to the statement ‘It’s a technical challenge to further process FDCA into value-added products’ (S07).

Most of the included papers which deal with FDCA synthesis use some form of HMF as starting material, either by creating it as an intermediate from a bio-based feedstock like starch, fructose, or glucose or by purchasing pure industrial HMF. Again, this result is supported by responses from workshop participants, who strongly agreed with the statement that ‘HMF is currently the primary starting material for FDCA production’ (S06). Indeed the ‘classical’ FDCA chain value starts from terrestrial plant-based sugars containing six carbons (i.e. fructose or glucose) that are dehydrated into HMF (or HMF-based ethers called RMF such as the methoxymethylfurfural). Then HMF or RMF are oxidized into FDCA. Basically, two main bottlenecks occur in this chain value. The first bottleneck is the formation of side-stream products in the intermediate production of HMF/RMF, such as levulinic acid (or levulinate esters) and humins. Levulinic compounds are single molecules

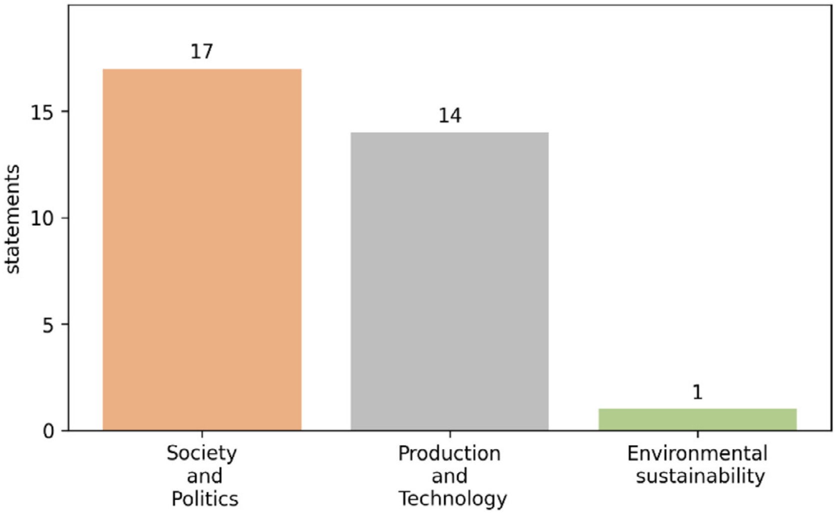

Fig. 8. Responses to the question on measures to reach the milestones, according to thematic clusters represented by the bars ($n = 19$ participants).

that can serve as solvents or platform chemicals for further derivatization; thus, their formation will have a limited impact on the HMF/FDCA value chain. On the other hand, humins are resinous or powder-like tarry polyfuranic macromolecules that are formed upon the condensation of HMF with residual sugars. Their yields can be important and can economically impact this peculiar value chain. This explains why major efforts have been recently been made to valorise humins in high-value added applications, as exemplified by the use of humins to impregnate wood cells, making wood timber more durable (e.g. Sangregorio et al. 2020), or to make sustainable foams (e.g. Chen et al. 2016a).

These considerations about side-streams products and also the overall HMF production process efficiency (such as catalyst recovery) would explain why the production of HMF is described as cost- and resource-intensive and not sustainable (e.g. Schade et al., 2019). Even the oxidation of HMF into FDCA leaves room for improved sustainability, according to Mei et al. (2015). In particular, the obligation to work with highly purified FDCA to avoid the future discoloration of FDCA polyesters (such as PEF) represents another bottleneck in the FDCA chain value. In addition, Motagamwala et al. (2018) note that, in order to be economically feasible, FDCA synthesis from HMF has to be carried out at high HMF concentrations. This fact is also noted by Hameed et al. (2020) who states that most of the reported studies with a high FDCA yield from HMF under aerobic oxidation conditions have been performed with diluted HMF. The use of diluted HMF, however, is not realistic for the practical production of FDCA on an industrial scale. According to Liu et al. (2020), the direct utilization of carbohydrate-derived crude HMF as a feedstock could be an intriguing alternative from an economic perspective, because the costly and difficult HMF separation/purification procedure could be circumvented. Unfortunately, impurities that arise when crude HMF or biomass are used as the starting material to create pure HMF and later FDCA increase the process inefficiency due to the lowered catalyst activity (Schade et al., 2019; Liu et al., 2020; Rathod and Jadhav, 2018). In this regard, Ogunjobi et al. (2019) also refer to catalysts as critical elements in FDCA synthesis due to their high economic value and the tendency to deplete if used continuously, as well as the fact that their supply could be restricted for geopolitical reasons. Moreover, HMF itself can currently only be produced to a limited extent from mono- and polysaccharides such as glucose and fructose, as noted by Shen et al. (2018), which is a barrier to the utilization of bio-based FDCA as a substitute for TPA in industrial applications.

Therefore, the choice of feedstock is a key consideration in that it determines the scale and efficiency of renewable resource-based processes (Schade et al., 2018). According to de Jong et al. (2012), it is also beneficial to use a strategy that allows great flexibility in obtaining feedstock for companies, requiring companies to consider factors ranging from the potential for sustainable production to the availability at the production site and on to the reliability of the logistics and general affordability.

The successful production of FDCA from lignocellulosic biomass has been demonstrated in studies like those by Zhang et al. (2015) or Jing et al. (2019). This literature review enabled us to identify a few more papers dedicated to FDCA synthesis from other starting materials than HMF (Ban et al., 2019; Shen et al. 2018). A different FDCA synthesis route is discussed in a handful of papers, the authors of which focus their attention on improving biotechnological approaches in this area. This is an emerging field that was also highlighted by workshop participants as being important. These publications describe how the researchers strive to find ways to synthesize FDCA using biocatalysts in multi- or single-stage (e.g. Hossain et al., 2017) processes, which can often be carried out under ambient conditions and avoid the high temperatures and pressures needed in most conventional processes (Lin et al., 2020). Furthermore, current biotechnological processes result in equally high FDCA yields (e.g. 94.2% in Chang et al., 2019) but produce less toxic waste (Lin et al., 2020). However, the reaction times for these processes were relatively long, ranging from about 10 hours (Wu et al., 2020) up to multiple days (e.g. Lin et al., 2020).

5.1. Economic aspects

Workshop participants identified several economic considerations, and in particular the price of FDCA, as being primary factors of the current challenges associated with bringing FDCA-based products to market Motagamwala et al. (2018). also notes that the only bottleneck in producing pure bio-based PEF is the lack of low-cost FDCA production. In the literature review, we identified some papers that address such techno-economic issues (Eerhart et al., 2015; Dessbesell et al., 2019; Triebl et al., 2013; Kim et al., 2020; Dubbink et al., 2021). Feedstock costs, catalyst costs, the selling price of FDCA and recovered catalyst, plant capacity, and the total investment were identified as the factors to which the economic feasibility of FDCA production was most sensitive.

Since FDCA is considered as a direct substitute for TPA, the price of FDCA should be competitive with or at best be below the price of TPA to facilitate its market entry. TPA is produced from fossil raw materials; thus, its price is strongly dependent on crude oil prices and subject to fluctuations. However, Dessbesell et al. (2019) give a range of $900 to 2200/t for the TPA price, citing Burry (2015) and Guzman (2012), whereas Motagamwala et al. (2018) assumed a value of $1445/t.

The workshop participants also mentioned economies of scale as a relevant factor in reducing production costs and supporting the commercialization of FDCA. According to Ghatta et al. (2019), the separation and purification steps in FDCA production are crucial for ensuring a possible scale-up of FDCA production.

Apart from TEAs, there is a lack of knowledge on other economic factors that are relevant for successful commercialization of FDCA/PEF, such as related to the broader (socio-)economic environment (actors, collaborations, company-level, etc.). Research efforts that contribute to a more holistic view about the underlying innovation system and sustainability by also including (broader) economic and social perspectives are thus urgently needed.

5.2. Sustainability aspects

Participants in the backcasting workshop also mentioned their concerns about the environmental sustainability of FDCA and FDCA-based products, indicating that they regarded these as an important factor affecting the market introduction. However, their statements were mainly related to end-of-life issues, such as the biodegradability of and difficulties associated with processing FDCA products together with already established materials in the existing recycling facilities. The reviewed literature, in contrast, indicated the necessity of taking a broader perspective such as including feedstock use (e.g., Álvarez-Chávez et al., 2012; Reichert et al., 2020), process level (e.g., Kümmerer, Clark, & Zuin, 2020; Álvarez-Chávez et al., 2012), and toxicity (Chen et al., 2016). Although literature suggests that environmental advantages of FDCA/PEF over TPA/PET seem possible (Eerhart et al., 2012) but cannot be taken for granted (Kim et al., 2020), participants focused on end-of-life issues only. This observation is perhaps in line with García González et al. (2018) who determined a reduction of 79% in greenhouse gas emissions in their LCA (furan-based polyester binder compared to its traditional fossil-based counterpart), but also noted that more in-depth research on the environmental burden of FDCA is still needed.

One noteworthy point is that the degradation behaviour of PEF may also cause a different sustainability issue regarding the formation of microplastic fragments; this concern stresses the importance of further research on degradation and end-of-life aspects once more (e.g., Maaskant and van Es, 2021; Siddiqui et al., 2021). While the primary use of FDCA to date is replacing TPA in PET, Ogunjobi et al. (2019) note that the influences of PEF in the existing PET recycling stream still need to be investigated. They suggest that a possible way to tackle furanoate in a terephthalate recycling stream could be by converting furanoate impurities in terephthalate streams to terephthalate itself, thus offering an alternative for chemical recycling. On the other hand, Avantium (2021b) indicates that PEF can be dealt with in the existing sorting processes, but only by using specialized equipment (i.e. NIR sorting equipment). PEF can be processed in the existing recycling streams with PET, but only with the interim approval from EPBP of up to 2%. The company also states that, due to its good barrier properties for carbon dioxide and oxygen, the use of PEF could also give packaged products a longer shelf life. In addition, this makes the production of a lighter bottle as compared to PET possible, which could save resources and transport cost (Avantium, 2021b).

5.3. Professional backgrounds and perceptions of the future

Given the scale of the current packaging market (as shown in Geyer et al., 2017), PEF has great potential as an end-use application. However, workshop participants responded neutrally to the statement that the demand for PEF will increase and that the market prospects are bright (S04). Although concrete ideas were apparent in the expressed future visions, and especially in relation to PEF (e.g. detailed shares with which PET could be replaced), the workshop participants also viewed the strong focus on PEF critically and pointed out that suitable niche applications for FDCA would also need to be explored. This observation could also be important for another reason, as PEF is considered to be the bio-based alternative to fossil-based PET, but recent advances have shown that the production of bioterephthalic acid is feasible, also making the production of bio-based PET possible (Chen et al., 2016b). In terms of alternative applications, the literature review results show that a wide range of applications for FDCA exist and that these applications are being explored.

An interesting shift in sentiment could be observed in the last part of the backcasting workshop. While the role of society and politics was found to be miniscule in the responses to the question about significant milestones, this role was mentioned as the most important lever to reach these milestones. This result indicates the respondents' perceived need for more regulatory measures like (fossil-based) plastic bans or levies (see, e.g UNEP, 2018.; Sousa et al. 2021), but participants also demanded more funding and consumer education. Communicating the benefits of FDCA to the consumers places a great demand on producers and value chain actors, requiring them to more clearly understand the consumers' needs (Karana et al., 2010). In this context, consumers are demanding more information about the environmental impact and expectations regarding the sustainability of these substitutes for fossil-based materials (Hesser, 2015; Ranacher et al., 2018), posing an additional challenge for their implementation.

From the perspective of the respondents/researchers, a detailed socio-economic approach will need to be taken to get FDCA into the markets, including a regulatory push rather than relying on the neo-classical economy (e.g. profit maximization) trust in a "perfect" market (e.g., Wenger et al., 2020 for lignin).

Workshop participants with a professional background toward the top end of the value chain referred more often to environmental aspects and ecological sustainability in their vision of the future. Furthermore, the result of the Pearson chi-squared test shows an interesting correlation between the answers given to the question about desired future visions of the experts. Participants with a professional background in technology development tended to refer to developments in the fields of markets and applications for FDCA in their future visions, while participants in the product development field tended to refer to technological aspects in their future visions. Thus, both of these groups tended to refer to developments in a field to which they did not assign themselves. This result indicates the limited view taken regarding the responsibility of stakeholders in the field of technology/industry/research, i.e. a bystander effect leads to inaction. This represents an easy argument for a person who does not need to implement these regulations.

This result also illustrates the fact that stakeholders, depending on their position in the FDCA value chain, have different perceptions regarding the future. It could indicate that industry experts should be included in research activities and vice-versa in an effort to tackle information asymmetries, as demanded by one workshop participant.

5.4. Limitations

The limitations of the literature review relate to the described keywords, the selected time frame and the selected database. The main limitation of the backcasting approach used in this study is that it had to be adapted for use in a time-limited online workshop. Nevertheless, it was possible to maintain the interactive character of the approach by using suitable tools, albeit making some compromises in terms of the methodological approach.

6. Conclusion

Although research on FDCA has been going on for many years, little commercialisation has yet taken place. Results of our literature review and backcasting workshop show that unlocking the full potential of FDCAs is restricted by several barriers, which are strongly related to technological and market aspects of the FDCA production. Considering the available literature, these barriers include the cost of the feedstock, but also the resources necessary for production, such as catalysts, solvents and energy demand, as well as the purity of FDCA. The same factors were identified as the biggest influence on the selling price of FDCA, one of the most important levers mentioned by the workshop participants for a successful market introduction. In economic studies, figures for a possible FDCA selling price have been provided, indicating that these fall within a competitive range with fossil counterparts like TPA.

While the workshop participants had specific future visions, most of which concerned PEF, the products discussed in the literature were more versatile and covered a wide array of niche applications. In the workshop, the highly divergent nature of the visions of the future described by the workshop participants became apparent. Participants with a background in FDCA production referred mostly to required developments in the field of FDCA applications in their desired future vision, while participants concerned with FDCA-product development mainly referred to open issues related to FDCA synthesis. This finding indicates that a great need exists for intensified cross-disciplinary communication and collaboration, supporting the value of large programmes such as FUR4Sustain COST Action.

While the currently developed plant for large-scale production of FDCA brings the market to the brink of the widespread availability of FDCA, the market for this promising molecule is still in its infancy. It remains unclear whether its price alone can enable the successful market introduction of FDCA (neo-classical economy), since the fossil-based production systems it competes against have been established for decades and operate by externalizing environmental costs. Hence, the role of society and politics in this regard was also emphasized by the workshop participants, who called for society members and policy makers to adopt legislation and provide more funding. An interesting finding is that the participating experts who had a predominantly technical background considered society and policy, in addition to production and technology, as key factors to achieving the desired visions. While further technological developments (e.g. upscaling, process efficiency) could result in production cost reductions, regulatory measures (e.g. carbon taxation, plastic ban, environmental promotion) could result in increased prices.

The study findings show that bringing FDCA products to market is an interdisciplinary process that requires corresponding interdisciplinary approaches. Techno-economic studies alone do not provide sufficient evidence for us to understand potential future pathways and the obstacles to reaching divergent visions.

Future research, therefore, could address uncertainties in the techno-economic area (e.g. feedstock, improvement of production processes, cost reduction, regulation), as well as those related to the environmental aspects of FDCA-based products. In addition, further research can promote cross-disciplinary collaboration, for example, by including perspectives from other decision-makers (e.g. policy makers, consumers).

Declaration of Competing Interest

The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.spc.2022.02.019.

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