Integrating ex-ante and prospective life-cycle assessment for advancing the environmental impact analysis of emerging bio-based technologies

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ABSTRACT

Unlike the fossil-based alternatives, many emerging bio-based technologies are still at the early lab or pilot scale and are not representative of optimized industrial conditions. This makes a robust comparison of their environmental performances via life-cycle assessment (LCA) challenging. We propose a framework to combine scaling-up projections of early-stage technologies (ex-ante LCA) with the influence of future socio-economic scenarios (prospective LCA), using a range of new bio-based polymers produced from forest residues as case study. The combined framework takes a step-by-step approach in modifying process inventories and projecting them to a future industrial scale for the environmental impact assessment. In our case study, the climate change impact from lab-scale processes decreases from 105–471 kg CO_2-eq./kg of polymer to 9–14 kg CO_2-eq./kg after the application of ex-ante LCA, with the highest reduction (83 %) coming from identified process synergies (e.g., solvent recovering). Combining the ex-ante and prospective LCA additionally reduces the impact up to 56 % by 2050, relative to ex-ante LCA results only. Other environmental impacts decrease as well, particularly freshwater eutrophication (up to 99 % reduction), photochemical oxidant formation (99 %), and marine eutrophication (98 %). The framework secures a more robust comparison of emerging bio-based products with conventional fossil-based alternatives, and as such it helps the identification of the improvements in both the bio-based technological processes and background supply chains that are needed to make bio-based systems outperform their fossil counterparts. A consistent integration of ex-ante and prospective LCA is instrumental to prioritize research and investments for upscaling the early-stage technologies that are most promising from a sustainability perspective, and ultimately guide a sustainable transition towards a circular bioeconomy.

1. Introduction

The global economy is mainly linear and heavily dependent on fossil resources. To achieve carbon neutrality targets and sustainable development goals, the society must move towards a circular economy relying on renewable resources. In the chemical sector, biomass is the promising renewable feedstock to replace conventional fossil-based polymers and reduce greenhouse gas (GHG) emissions (Meys et al., 2021; Zheng and Suh, 2019). Currently commercialized bio-based polymers typically suffer from limited processability and low glass-transition temperature (Rosenboom et al., 2022; Nguyen et al., 2018), and they are mostly used for applications where the requirements for material properties are low. Easily processable bio-based polymers that maintain adequate thermal and mechanical properties at higher temperatures, are highly demanded in the automotive, construction, coating, and packaging sectors (Nguyen et al., 2018). Currently, however, the processes leading to such high-performance bio-based plastics are still often under development at the lab scale and low technology readiness level (TRL) (Bonjour et al., 2021; Galbis et al., 2016; Laanesoo et al., 2021). Not only a proper assessment of their environmental impacts is challenging, but also their

early-stage performance and impacts cannot be fairly compared with optimized commercial fossil alternatives (Thonemann and Schulte, 2019; Thonemann et al., 2020), thus preventing the identification of the most sustainable options. Scaling-up laboratory and pilot data of bio-based polymers production to a commercial scale is instrumental to identify environmental hotspots and bottlenecks (Ögmundarson et al., 2020) and guide their development from a techno-economic and environmental point of view from the early stages of design (Liang et al., 2023).

As conventional life-cycle assessment (LCA) has limitations in the environmental impact assessment of developing technologies, more advanced approaches such as ex-ante and prospective LCA have been identifying the most promising bio-based options and their opportunities for improvements. Ex-ante LCA is a term that usually indicates an approach to scale-up low TRL technologies to explore their potential environmental performance in a higher TRL situation, so they can be consistently compared with commercial alternatives in a more adequate manner (Cucurachi et al., 2018; Moni et al., 2020; van der Giesen et al., 2020). Prospective LCA is another term that in some context compares technologies at different times (i.e., future scenarios) and can be applied to both emerging and commercial technologies (Thonemann et al., 2020; Arvidsson et al., 2018). Ex-ante LCA is based on the scaling-up of foreground data (frequently available at a lab or pilot scale) via multiple possible methods, including process-based simulations (i.e., using models and software) or calculations (i.e., using equations projecting mass and energy balances) (Piccinno et al., 2016), definition of scenarios of large-scale production by means of experts' interviews (Arvidsson et al., 2018) or ranges (Cucurachi et al., 2018), and application of scaling factors and learning curves (Zhou et al., 2017; van der Hulst et al., 2020). In prospective LCA, background data are changed according to future technical and socioeconomic developments using predictive scenarios (Arvidsson et al., 2018; Thonemann et al., 2020) and the integration of the future changes relies on projections from Integrated Assessment Models (IAMs) (Joyce and Björklund, 2022; Sacchi et al., 2022; Mendoza Beltran et al., 2020). These projections reflect changes in our socioeconomic system in conjunction with various climate change policies, providing multiple socioeconomic narratives of alternative future scenarios. For example, our energy production and consumption gradually become more decarbonized while approaching climate change mitigation targets thanks to improvements in electricity production mixes (i.e., less use of fossil fuels and increased use of renewable energy), power plant efficiencies, transportation fleet and energy mix, among others (Sacchi et al., 2022; Lamers et al., 2023).

Despite increasing efforts to harmonize LCA of emerging technologies (Tsoy et al., 2020; Arvidsson et al., 2018; Thonemann et al., 2020), different definitions of ex-ante and prospective LCA than the ones given above are common, thereby hindering comparability among studies (Moni et al., 2020; van der Giesen et al., 2020). Ex-ante and prospective LCA definitions can be overlapping (Moni et al., 2020) and often ex-ante LCA is considered a subset of prospective LCA (Thonemann et al., 2020). When definitions are not clear, effects from gradually scaling-up the maturity level of the technology and those from the future changes in the background economy can be hardly distinguished, and the analysis does not transparently inform about the specific contributions that can be expected from each of the two. This limits an understanding of how much improvements can be expected by developing an early-stage technology to an industrial scale, from the improvements that will come from market dynamics that are external to the system. A stepwise approach where these different methods are implemented would be beneficial to harmonize scientific literature, improve comparison across studies, and facilitate identification of methodological improvements, ultimately making LCA a more robust tool to assess environmental performances of early-stage technologies and support prioritization of R&D strategies.

In this study, we propose a combined framework to perform a fair benchmark of novel bio-based technologies against their fossil counterparts by clearly defining and separating ex-ante and prospective LCA and introducing a transparent stepwise approach for their implementation. Using a production system of bio-based chemicals still at a low TRL as a case study, we explore how LCA results vary by gradually implementing ex-ante and prospective LCA. The bio-based polymers are produced from forest residues and represent a circular bioeconomy system that can potentially replace conventional plastics in sectors with currently no renewable alternatives. The case study comprises countries with either a clean (Norway) or more carbon intensive (Estonia) electricity mix. The European Union (EU) electricity mix is also included to represent average conditions.

2. Methods: combined framework

The proposed framework to assess the environmental sustainability of bio-based emerging technologies combining ex-ante and prospective LCA is summarized in Fig. 1, and it is inspired by a review of existing studies that applied these approaches to assess emerging technologies (Table S1, Supplementary material). This framework is applied to a case study, detailed in Section 2.4. First, ex-ante and prospective LCA are classified according to their temporal dimension and TRL to which they apply (Fig. 1a). Then, their integration is divided into three main phases (Fig. 1b): Phase I: goal and scope definition, Phase II: scaling-up foreground data, and Phase III: projecting background data.

Phase I brings elements from van der Hulst et al. (2020) and Thonemann et al. (2020), such as the importance of defining the functionality and system boundaries for a better comparability of the emerging technology with the conventional counterpart. Phase II focuses on ex-ante LCA, and it includes the scaling-up of lab-scale technologies, and it can be implemented through six parts undertaken in continuous dialogue with the technology developers: process description (I), plant flow chart (II), process synergies (III), improved yields (IV), side stream (V), and scale-up to industrial scale each identified process step (VI). This approach is similar to the one developed by Piccinno et al. (2016), which includes a breakdown into laboratory protocol, plant flow chat, scaling-up of each process step, linkages and synergies. Our method is expanded to explicitly consider the modelling and characterization of process yields and side-streams (key performance indicators) and emphasizes the constant communication with the developers. Phase III implements the prospective LCA by projecting background data according to future scenario narratives and climate change mitigation targets (Sacchi et al., 2022). This approach is similar to what proposed in other studies (Ballal et al., 2023; Watanabe et al., 2022), but they so far did not consider its application to scaled-up foreground data and integration with ex-ante LCA, as explored in our analysis. Finally, an uncertainty analysis is performed, as recommended by Thonemann et al. (2020).

2.1. Phase I: goal and scope definition

In Phase I, the goal and scope of the assessment are defined by selecting the emerging technology, key methodological aspects, and its TRL.

2.1.1. Identification of counterparts

For benchmarking the environmental benefits of the emerging bio-based technology, it is essential to identify the commercial (fossil) counterpart(s) that the novel products could replace. The benchmark with counterparts establishes the necessary improvements (e.g., higher yields and minimum thresholds of efficiency) and highlights the advantages of the bio-based alternatives with the same functionality, but lower environmental impacts. This identification is not always straightforward, especially because a one-to-one replacement is not always possible and because the reference system can be dynamic and change in the future (e.g., in the case of average electricity mixes). Case-specific considerations are to be undertaken, and ideally more than one counterpart can be identified and/or explored.
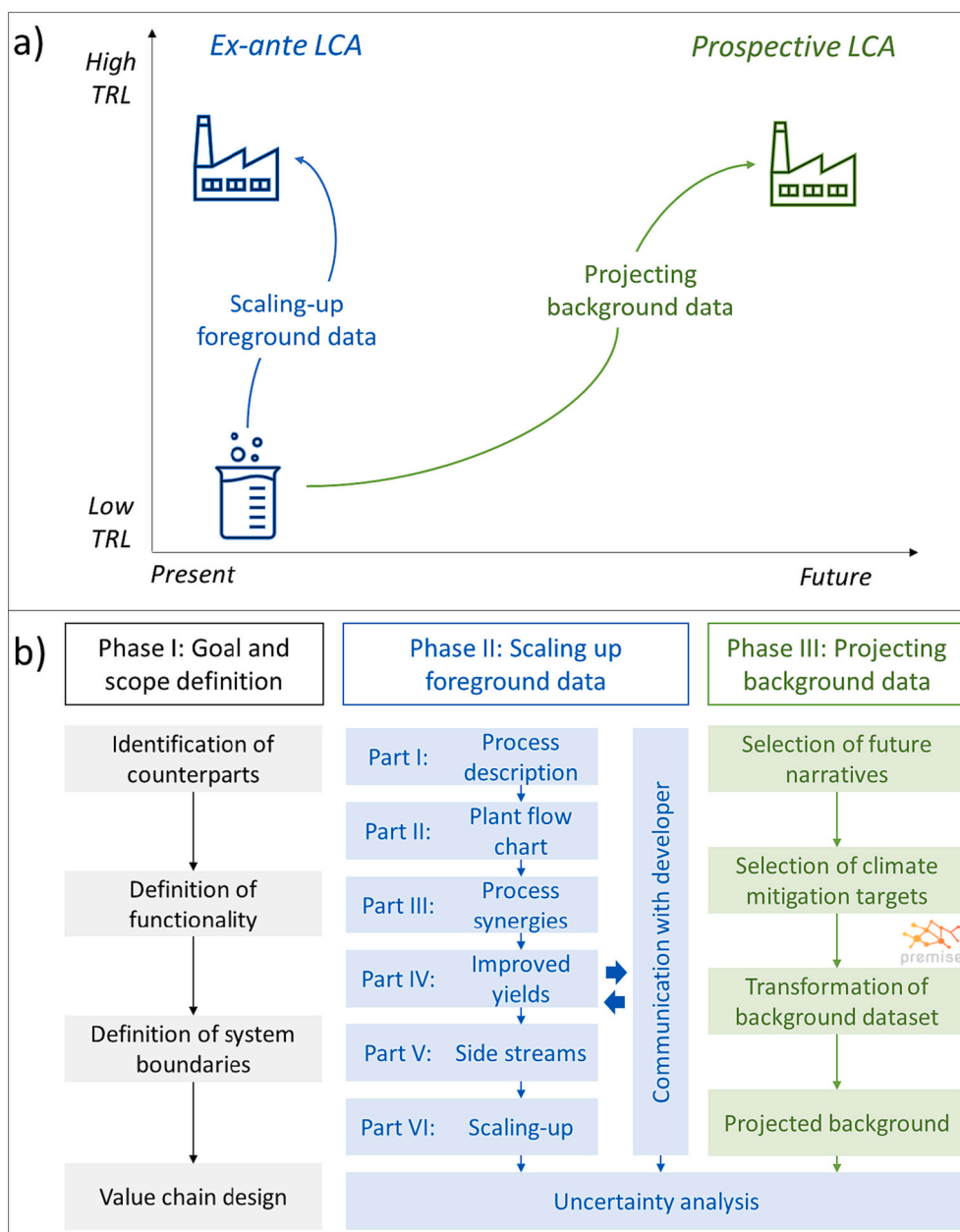
Fig. 1. Integration of ex-ante and prospective life cycle assessment. Representation of the differences in temporal dimension and TRL (a), and proposed process steps required for the integration, grouped into three main phases (b).

2.1.2. Definition of functionality

Bio-based chemicals and polymers can be drop-in or dedicated. The drop-in ones provide the exact same structure, properties, and functionality as the fossil counterparts (e.g., bio-based polyethylene). The dedicated ones are not always a direct replacement for their conventional counterparts. They can provide different chemical and mechanical properties (e.g., polylactic acid), and deliver new functionalities and services, including improved biodegradability, and lower toxicity (Zheng and Suh, 2019). These aspects challenge the definition of a function unit (Moni et al., 2020; van der Giesen et al., 2020). For a general application, the functional unit can be the mass of polymer produced (i.e., 1 kg of polymer), while for more specific applications it can be units of the specific product, for example 1 plastic bottle, 1 packaging container, etc., or it can consider the impact (i.e., 1 kg of plastic waste).

2.1.3. Definition of system boundaries

The system boundaries consider the main life-cycle stages of the technology and explore realistic value chains that can supply the required biomass. Ideally, the local availability of residues should be compared with the intended size of the plant, and supply chains from either residues or new biomass streams should be compiled for comparative analysis. A cradle-to-grave approach should identify all potential environmental impacts the new product may result until its end-of-life (Thonemann et al., 2020). This is particularly important for bio-based technologies. In general, the end-of-life adds extra impacts in the case of fossil-based products as they release fossil CO_2, so the bio-based options generally perform better, as their carbon content is biogenic. The potential CO_2 emissions are from the biomass growing cycle or it contributes to temporary carbon storage and potential negative emissions (Stegmann et al., 2022). The latter happens when the product remains sometime in the anthroposphere as stocks or is recycled into new products multiple times before its oxidation back to CO_2.

However, fossil carbon released as CO_2 contributes to long-term and irreversible climate change, and its temporary storage before oxidation does not contribute to climate benefits.

2.1.4. Value chain design

Based on the previous definitions, a value chain is designed considering all life cycle stages associated with the emerging technology, i.e., biomass feedstock selection and production, transport, and conversion to intermediate and final products, use phases and end-of-life. Appropriate assumptions and scenario analysis of transportation systems and end-of-life treatments should consider the specific context where the system will be implemented.

2.2. Phase II: ex-ante life cycle assessment

In Phase II, foreground systems containing laboratory data of mass and energy balances of the novel technologies are scaled-up to higher TRL by implementing six steps, which should be developed in continuous dialogue with technology developers, whenever possible (Fig. 1b).

2.2.1. Part I – process description

A process description based on the laboratory protocol is designed by making an inventory of the main inputs, yields, and mass and energy balances. During this part, the production process is divided into main reaction steps based on the identified lab-scale procedures, with an attribution to each step of the materials and equipment, with a first screening of what is relevant and needs scaling-up and what is only valid for lab experiments and has to be removed when projecting the process at an industrial scale. Some lab routines and specific purification methods are not likely to happen in an industrial scale and can be taken out. These may involve high-impact chemicals and materials, that will be most likely replaced or removed at a commercial scale.

2.2.2. Part II – plant flow chart

A plant flow chart is designed with all process steps, reactors, auxiliary inputs, machinery, and equipment required for each operation unit of the process. This flow chart illustrates the main steps of the production process and is the basis of the scaling-up procedures (Part VI).

2.2.3. Part III – process synergies

The potential process synergies are identified after having the definition of the process description and the plant flow chart. They include options for material recovery (e.g., chemicals, solvents, reactants) and energy recovery (i.e., heat integration). This step removes or replaces the lab-scale procedures identified as redundant during the process description (Part I).

2.2.4. Part IV – improved yields

In lab-scale procedures, the reagent stoichiometry and solvent use are not usually optimized, resulting in relatively high volumes of waste products. Projections of optimized yields and higher efficiencies at industrial scales can be achieved by considering stoichiometric optimal overall yields and/or ranges of plausible yields (close to maximum theoretical yields) (Langhorst et al., 2023).

2.2.5. Part V – side streams

Side streams (e.g., co-products, fugitive emissions, and residues) can also be stoichiometrically adjusted after yields are optimized. Identifying co-products with commercial usability can also reduce the impacts attributed to the main product and improve the overall environmental and economic performances of the system. An initial mapping and understanding of the potential most toxic fugitive emissions and hazardous residues, on the other hand, can lead to an early understanding of the main possible challenges with opportunities for identifying mitigation and/or measures remediation (e.g., downstream abatement or proper waste handling) before the pollutants are released to the environment.

2.2.6. Part VI – scaling-up

Each main step of the production process identified previously is scaled-up separately, applying equations, estimations, and assumptions, e.g., as those based on Piccinno et al. (2016, 2018) applied at laboratory or pilot scale. Energy requirements, usually not considered in laboratory protocols, are estimated including energy demands for recovery of chemicals, eventual heating, stirring, distillation and/or filtration.

2.3. Phase III: prospective life cycle assessment

Emerging bio-based technologies will need at least a decade before becoming commercially available, and their environmental impacts should therefore consider the possible technical and socioeconomic changes of these years. For example, rapid changes in the electricity production mix and transport systems impact the indirect emissions.

2.3.1. Selection of future narratives and mitigation targets

Prospective LCA can integrate alternative future socioeconomic scenarios from IAMs in the LCA background data (Sacchi et al., 2022), providing a representation of future changes in the context of the Shared Socioeconomic Pathways (SSPs) (O'Neill et al., 2017; Riahi et al., 2017). The SSPs combine various social, economic, and environmental changes (e.g., energy production, transport sector, and society, environmental policies, etc.) (O'Neill et al., 2017).

The SSPs can be combined with various climate change mitigation targets or emission reduction pledges, such as the Representative Concentration Pathways (Riahi et al., 2017) or the Nationally Determined Contributions in the Paris Agreements (Roelfsema et al., 2020).

2.3.2. Transformation of background dataset and projections

The transformation of the LCA background dataset to embed these scenarios is a rapidly evolving field, with significant contributions and achievements in recent years. PREMISE is a software package that can transform Ecoinvent database activities (mainly related to electricity, cement, steel, fuels, and transportation modals) into future processes in line with IAM-based scenarios (Sacchi et al., 2022). The transformed background dataset is connected to the foreground inventories to perform the impact assessment within a consistent future setting.

2.3.3. Uncertainty analysis

Finally, parameters that include variability in key factors connected with the combined framework to simulate higher technological maturity and a complete value chain should be defined for an uncertainty analysis. It strengthens the robustness of the results and help to achieve a better interpretation (Moni et al., 2020; Thonemann et al., 2020).

2.4. Case study: bio-based polymers from forest residues

2.4.1. Goal and scope definition

We apply the combined framework to assess environmental impacts of an idealized biorefinery system based on emerging technologies at a laboratory scale (TRL 4) and provide a comprehensive stepwise assessment for climate change impact. This case study addresses the fossil chemicals for which there are currently no commercial bio-based alternatives available and are therefore among the most challenging to target for the reduction of our dependence on fossil sources. An early-stage assessment of the possible bio-based emerging technologies to produce these chemicals is thus needed to explore the potential benefits.

The biorefinery converts forest residues into three bio-based polymers, isosorbide-derived PIMA, vanillic acid-derived PVAMEMA, and unsaturated polyester resins (UPR), a polymer partially made from maleic anhydride (MA), obtained via furfural (Fig. 2; a more detailed diagram is provided in Fig. S1). Isosorbide, vanillin, and furfural, the precursors of these bio-based polymers, are obtained from cellulose,
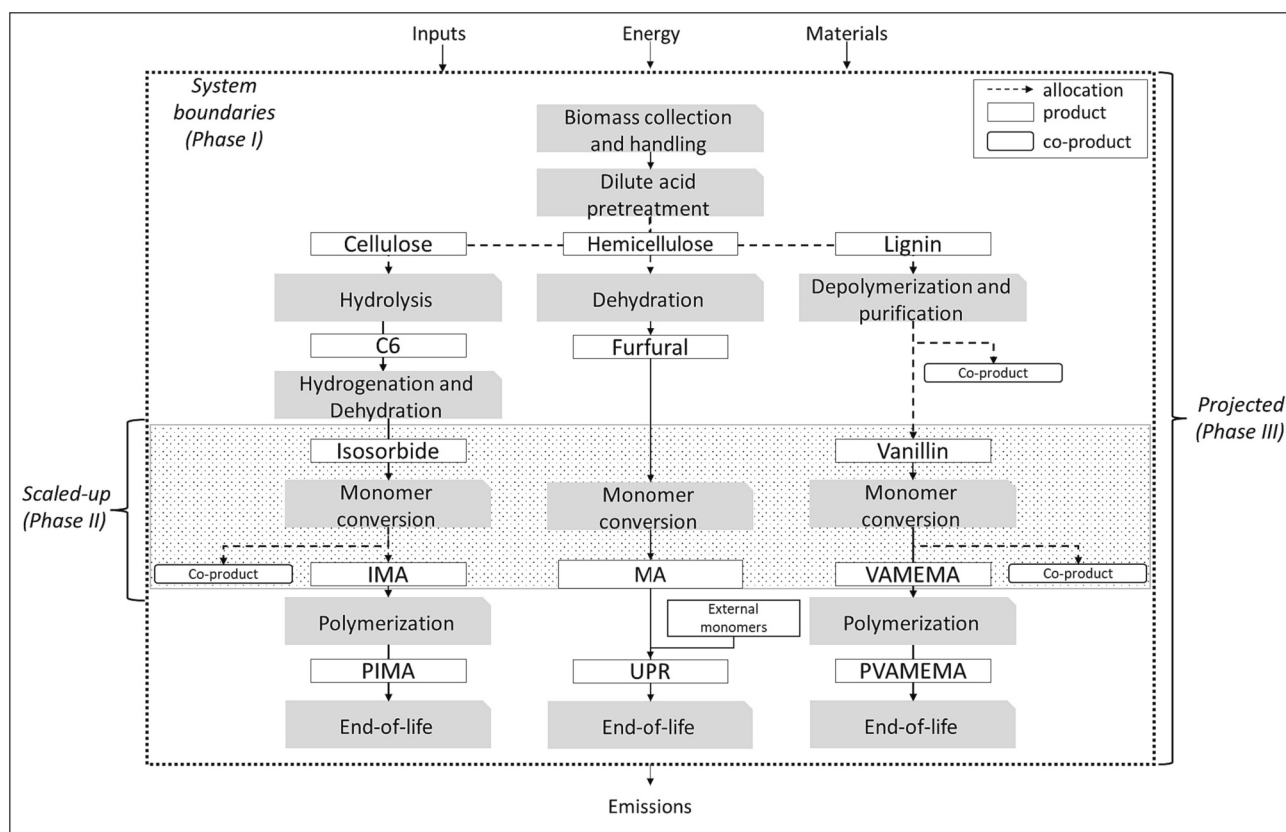
Fig. 2. Schematic diagram of the biorefinery system producing bio-based polymers from forest residues.

lignin, and hemicellulose, respectively. PIMA and PVAMEMA have high glass transition temperatures (Matt et al., 2018, 2021, 2023) and characteristics similar to fossil polystyrene (PS), poly-methyl methacrylate (PMMA) and polycarbonate (PC), currently widely used fossil-based counterparts. The alternative for the furfural-derived UPR is the fossil-based UPR. Around 38 % (mass basis) of UPR is composed of MA, and the remaining content is made of fossil-based chemicals such as diethylene glycol, ethylene glycol, styrene, and propylene glycol (Moreno Ruiz et al., 2021). An overview of the bio-based monomers, polymers and their fossil alternatives are available in Table S2 and Fig. S2.

The biorefinery system is designed in a cradle-to-grave approach, accounting for inputs and emissions from forest residues collection, handling, storage, and transportation to the biorefinery, biomass conversion to the intermediate chemicals and to the targeted bio-based polymers, and their end-of-life treatment. The functional unit is 1 kg of polymer. The assessment considers three different locations (Norway, Estonia, and average European Union conditions) representing somewhat different biomass composition, grid electricity mix and transportation distances (see Supplementary Table S3). Norway has a considerably high proportion of clean electricity in its mix with 87 % of hydropower (SSB, 2023a), while Estonia has only 29 % of electricity from renewable sources (Statistics Estonia, 2023). The associated average GHG emission per unit of electricity produced are 19 g CO_2-eq./kWh in Norway, 388 g CO_2eq./kWh in the EU, and 870 g CO_2eq./kWh in Estonia (Moreno Ruiz et al., 2021).

The inventories are created by gathering primary data from existing studies for the feedstock collection and conversion up to the intermediate chemicals (i.e., isosorbide, vanillin and furfural) and from laboratory protocols for the synthesis of these chemicals (Supplementary Table S4). For PIMA and PVAMEMA synthesis the lab inventories for mass and energy balances, yields, emission factors, co-products, and prospective polymers are collected directly via close dialogue with the chemical experts that conducted the lab experiments.

Electricity requirements are considered to be directly taken from the national grid (Norway, Estonia, or the EU average) while the required process heat is produced from combustion of wood residues. The forest residues are considered without any upstream impact burden, except for their collection and transportation to the biorefinery plant. GHG emissions from storage and chipping of forest residues are based on Morales et al. (2021). Dilute acid pretreatment (Morales et al., 2021) is applied to decompose lignocellulosic biomass into cellulose, hemicellulose, and lignin, and emissions are allocated on a mass basis (Supplementary Table S3). After the pretreatment, the cellulose stream is hydrolyzed into glucose (Morales et al., 2021), which is then converted to sorbitol via hydrogenation (Moreno et al., 2020) and subsequently dehydrated to isosorbide (Kamaruzaman et al., 2020). Xylose is dehydrated to furfural in the presence of an acid (Lin et al., 2015). The lignin stream goes through a depolymerization step to obtain purified vanillin (Khwanjaisakun et al., 2020). The vanillin conversion to vanillic acid is omitted from our analysis due to a lack of data.

The lab-scale conversion process from isosorbide to isosorbide-monomer (IMA) involves two synthetic steps: methacrylation and acetalization (Laanesoo et al., 2021). The vanillin-derived monomer (VAMEMA) is synthesized in two steps, and the data are based on lab-scale experiments. The conversion of furfural to MA is relatively simple and involves catalytic oxidation of furfural in the gas phase (Li et al., 2016). The detailed mass balances are provided in Table S5, and the scaling-up of lab-scale foreground data is discussed in the next section.

As the IMA and VAMEMA monomers can be polymerized under standard polymerization conditions routinely used also for fossil references PMMA and PS, the polymerization impact was estimated to be 1.0 kg CO_2-eq./kg bio-based polymer, which is the average value for the polymerization of MMA and styrene (see Table S6). The polymerization of furfural-derived UPR was modelled replacing the conventional MA with the bio-based one, resulting in 0.5 kg CO_2-eq./kg UPR (Table S6).

Incineration is the most common end-of-life treatment of PS, PC, and

PMMA wastes in Europe, Norway, and Estonia, thus we considered a 100 % incineration rate. Although 53 % of Norwegian plastic waste ends up in recycling stations and 43 % goes directly to incineration (SSB, 2023b), durable products containing PC, PMMA, PS, and UPR represent a small share of plastic waste and currently are not recycled, but incinerated (Furberg et al., 2022). In Estonia, 42 % of plastic waste is incinerated and 32 % of plastic waste goes to landfills (Eurostat, 2023), but the considered polymers are not biodegradable and possible plastic litter is not included in this study's scope. Most of the carbon content of the bio-based polymers originates from biomass (i.e., isosorbide, vanillin, and furfural), and is considered biogenic, while the rest is of fossil origin due to the use of reactants and additives. The share of biogenic carbon content is calculated according to the carbon balance provided in Table S7, and it is used to estimate the biogenic or fossil CO_2 emissions from incineration. Fossil CO_2 (and other GHGs from the value chain) are assessed with the 100-year global warming potential (GWP100) (IPCC, 2013). Impacts on fossil depletion, freshwater eutrophication, human toxicity, marine eutrophication, ozone depletion, and photochemical oxidant formation are assessed using ReCiPe 2016 impact categories (Huijbregts et al., 2017).

2.4.2. Application of ex-ante LCA

Not all the value chain needs the application of ex-ante LCA, but only the bio-based monomer production that is currently at a low TRL and requires scaling-up its production system to estimate the environmental effects at an industrial scale. A detailed summary of the application of all Phase II parts and respective outcomes is provided in Table S8.

In Part II, the flowchart was designed selecting the necessary equipment and machinery for each operation unit. For example, all three monomers require reactors with heating and stirring. The flowchart is presented in Fig. S3.

In Part III, based on a discussion with the chemical scientists developing the experiments in the laboratory, a 97 % recovery rate is assumed, since the recovery process is relatively simple, and the chemicals are not contaminated. The technological developers expect to reuse the catalyst up to ten times in the synthesis of MA (Li et al., 2016), which is the value considered in our analysis. Stabilizers and some of the washing steps, not typically applied at industrial scales, were removed. At the lab-scale, the solvents, and chemicals to produce PIMA and PVAMEMA are used in high amounts and discarded, but at the industrial level, they are recovered and reused.

In Part IV the potential of optimized yields is explored by considering that all reactants (i.e., isosorbide, furfural, and vanillin) are transformed into the targeted compounds, at the maximum conversion efficiency. An optimized yield for lignin depolymerization into vanillin was also considered, achieving a 60 % higher overall yield (Wang et al., 2018), than what was observed at lab-scale. In Part V, in dialogue with the chemical experts, acetic acid, acetaldehyde and methacrylic acid were identified as co-products for isosorbide and vanillin monomers as they all have a market value (Biddy et al., 2016; Taylor et al., 2015) and could be easily isolated during the reactions. No co-products are generated during the conversion of furfural to maleic anhydride. Side streams are also identified for the depolymerization of lignin into vanillin, and environmental impacts are allocated to sodium sulfate, a co-product with commercial value. Allocation values to co-products are provided in Table S9. No hazardous residues and wastes or fugitive emissions were identified.

In Part VI, the required energy for heating and stirring the reactions, recovery of chemicals, filtration, centrifugation and to integrate the process (e.g., pumping) is calculated applying Eqs. (S1), (S2) and (S3) and Tables S10 to S13 (available in the Supplementary material), based on Piccinno et al. (2016).

2.4.3. Application of prospective LCA

The prospective LCA is applied by projecting background data using PREMISE version 1.2.5 (Sacchi et al., 2022). This code package transforms the Ecoinvent 3.8 database (Moreno Ruiz et al., 2021) into future background systems provided by IAM scenarios.

For the selection of future narratives, we used projections from the model REMIND (PIK-Postdam, n.d.) for the SSP2 – Middle of the Road (Fricko et al., 2017). SSP2 is not only an extrapolation of current trends but includes historical patterns such as emerging economies growing quickly and then slowing down after reaching higher income levels, and uneven growth patterns among countries (Fricko et al., 2017).

The selection of climate mitigation targets considers the climate policies of the Nationally Determined Contribution (NDC) for Europe, Norway, and Estonia. The SSP2-NDC is a scenario where countries implement existing pledges and emission reduction targets as submitted to the Paris Agreements, consistent with a global average temperature rise of about 2.5 °C by the end of the century.

The transformed background datasets are the ones included in the default transformation of PREMISE after coupling with IAM projections (power generation, cement production, steel production, transport, and fuels) (Sacchi et al., 2022). The main changes are related to efficiency improvements and addition of new technologies (e.g., cleaner energy sources, biofuels, carbon capture and storage, etc.). Further details are provided in Table S14. To this, we further add transformations that are relevant to our case study, such as an additional disaggregation of the electricity mixes for Norway and Estonia (as IAM only has future projections averaged at European level), and the future availability of bio-based chemicals that can be used as reactants instead of fossil-based chemicals in our process technology.

Regarding electricity, the IAM REMIND has a low disaggregation level for country climate policies at the IAM geographical coverage, and Europe is considered a single economic block. We thus estimated the future electricity mix in Norway based on Norwegian projections (Det Norske Veritas, 2020) and in Estonia based on the disaggregated country-specific electricity mix generated by PREMISE. A summary of the evolution of the electricity mixes in the two countries is shown in Table S15.

Regarding bio-based chemicals, PREMISE currently reduces the indirect emissions associated with the production of chemicals as a result of cleaner background energy and transport systems, but it does not change the primary feedstock, meaning that in the future the chemicals will still be sourced from fossil fuels, even under the implementation of strict climate change mitigation policies. The selected bio-based polymers in our case study still require a certain amount of fossil chemicals as reactants and during the monomer synthesis. This has an effect particularly for the end-of-life when incineration releases fossil CO_2 to the atmosphere. In the prospective LCA, we thus implement a change in the chemical sector implementing a fully biogenic carbon content of the bio-based polymers by 2035 and 2050. Although this might be an optimistic scenario, it is consistent with a de-fossilization trend as intended with the NDCs and it provides a benchmark of the possible benefits that our early-stage technology can achieve from a large-scale availability of bio-based chemicals replacing fossil-based chemicals.

2.4.4. Uncertainty analysis

Finally, the robustness of the combined framework applied to our case study is assessed through a Monte-Carlo analysis that investigates the propagation of uncertainties of significant decisions and assumptions taken to scale-up the lab-scale data to a higher maturity level. A Monte Carlo analysis is run with 10,000 iterations in a triangular distribution considering upper and lower values in key uncertainty factors as detailed in Table S16. Most of these ranges were determined in dialogue with the chemical experts. The triangular distribution is chosen according to the principle of maximum entropy (adapted from Mishra and Datta-Gupta, 2018 and Van der Spek et al., 2020), which fits better when we know the minimum, maximum, and mode values of each parameter, rather than a lognormal distribution that is more commonly used in LCA when the uncertainty range of the values is less constrained (Ravetz and Funtowicz, 1990; Ciroth et al., 2016).

3. Results

3.1. Ex-ante LCA

An LCA applied to the novel bio-based chemicals directly using lab-scale data within a value chain perspective led to climate change impact in the range of 105–471 kg CO_2-eq./kg polymer (Fig. 3), with the European electricity mix. These values are considerably higher than fossil-based reference polymers PMMA, PS, PC and UPR (6 to 11 kg CO_2-eq./kg polymer), which take advantage of industrial production scales and optimization. The progressive consideration of ex-ante LCA measures, reduced the range of impacts to 9–14 kg CO_2-eq./kg polymer. GHG emissions were reduced by around 91 % for the isosorbide polymer (PIMA) (Fig. 3a), 97 % for vanillin-derived polymer PVAMEMA
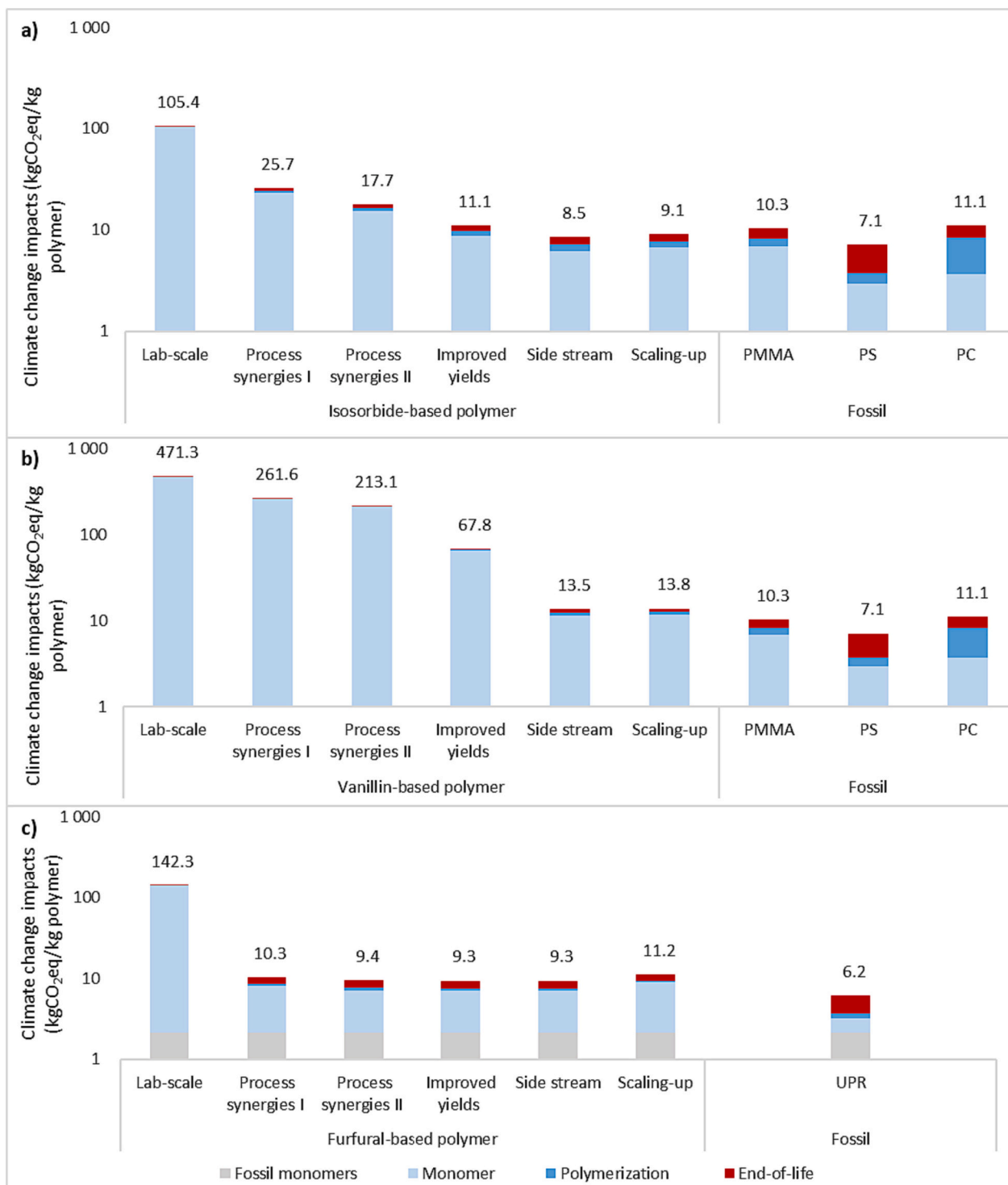
Fig. 3. Impacts of prospective LCA on a) isosorbide-derived PIMA; b) vanillin-derived PVAMEMA; c) furfural-derived UPR, compared to their fossil alternatives. EU electricity mix is considered. Lab-scale: mass balances and inputs from laboratory protocol. Process synergies I: Recovery of the main solvent; Process synergies II: Recovery of other chemicals; Improved yields: no reactant wastes, at maximum product yield. Side streams: identified co-products with allocation of impacts. Scaling-up: required energy and its indirect emissions for monomers conversion stage. For better visualization of the wide range of values, y axis is on a logarithmic scale.

(Fig. 3b), and 92 % for furfural-derived UPR (Fig. 3c), relative to the initial lab-scale data.

The application of the Part III (i.e., process synergies) caused the largest reduction in the life-cycle climate change impact. This is primarily due to the recovery of the main solvent (process synergies I in Fig. 3), followed by the recovery of other chemicals (process synergies II in Fig. 3). For the synthesis of IMAs and VAMEMA, ethyl acetate is the main solvent that can be recovered, while for MA, it is an acetic acid. Setting up a 97 % recovery rate and a 100 % overall yield is ambitious, but it shows the extent of improvements needed to perform equally or better than conventional fossil alternatives. The communication with chemists undertaking the lab experiment is key in this Part, as they indicated that the solvents can be easily recovered via evaporation or distillation and no contamination occurs. However, in some other bio-based processes than this case study, contamination and/or complex separation could make the recovery unfeasible from a techno-economic perspective, thereby reinforcing the needs for case-specific analysis and expert engagements.

Improving the yields (Part IV) reduced the impacts of PVAMEMA by 32 %. The lab-scale overall yield for lignin depolymerization into vanillin and vanillin conversion to VAMEMA is only 8 % and 46 %, respectively. This step shows the importance of considering higher yields of low-TRL processes in ex-ante LCA to achieve more realistic estimates of industrial scale conversion efficiencies. For PIMA and UPR, which originally have considerably higher overall yields (86 % and 93 %, respectively), Part IV reduced impacts by less than 7 %.

The target product has very low overall yields in many bio-based production processes, and several other compounds are generated during the conversion. In this case study, the identification of side streams and co-products (Part V) reduced PVAMEMA impacts by 12 %. The lignin depolymerization into vanillin generates large amounts of sodium sulfate, which has commercial value. For PIMA, the generated co-products also have commercial value, but only account for 3 % of impact reduction as their amounts are not as significant as the vanillin case.

In Part VI – scaling-up, the estimated indirect emissions for the energy needs of the scale-up system had no significant impact on the overall GHG emissions (i.e., 0.3 to 1.9 CO_2-eq./kg polymer), because the syntheses of monomers in this case study are mostly performed at room temperature and the recovery of chemicals is not energy intensive. In other contexts, and for different emerging technologies, this issue could be an environmental hotspot.

After scaling-up, the bio-based polymer from isosorbide (PIMA) is a potential replacement for fossil-based PMMA and PC; however, fossil PS emits about 22 % less GHG emissions per kg of polymer (Fig. 3a). The system boundary definition (Phase I) considering a cradle-to-grave approach that includes polymerization of the monomers and the end-of-life treatment (100 % incineration in EU) is key to benchmark the bio-based polymers with their fossil counterpart. However, even when considering the end-of-life benefits of bio-based polymers (i.e., biogenic carbon content), PVAMEMA and furfural-derived UPR present higher emissions than their fossil equivalents (Fig. 3b and c), showing that further improvements are necessary, beyond the ones considered in this ex-ante LCA.

Potential further improvements for PIMA and PVAMEMA include replacing fossil-based reactants (i.e., acetic anhydride, methacrylic anhydride, vinyl methacrylate, methanol) with bio-based ones; methacrylic acid generated during the monomer conversion could be either converted back to methacrylic anhydride and reduce its input in the process, or directly used as a reactant, but more tests are needed. The granulated immobilized enzyme catalyst from IMA conversion step has the potential for reuse (at least ca five times), but we have taken a conservative approach and assumed no reuse in this study. For bio-based MA, improving furfural conversion, reducing solvent amounts and multiple reuses of the catalysts are necessary to result in lower climate change impact than the fossil equivalents. An energy integration could

improve the biorefinery efficiency, mainly for the lignin depolymerization to vanillin, the cellulose conversion to sorbitol, and the subsequent dehydration to isosorbide, and import less heat and electricity from the grid. Another option is to divert part of the forest residues to provide heat and power in a cogeneration system. Some of these improvements are included in the uncertainty analysis and are presented in the next section. But not always uncertainty analysis is sufficient, and sensitivities should be considered. For the case of PIMA, alternative pathways based on Matt et al. (2018) and Gallagher et al. (2015) are considered in a sensitivity analysis and the results are presented in Table S17.

3.2. Prospective LCA and uncertainties

The combination of ex-ante with a prospective LCA reinforces the climate benefits of the bio-based options. The prospective results consider a future context of climate action with countries successfully mitigating their GHG emissions according to their existing NDCs and assuming that in 2035 and 2050 all carbon content in bio-based polymers (Table S7) will be biogenic or produced from low carbon renewable resources. Climate change impact are reduced by 30 % to 42 % from 2020 to 2035, and by 31 % to 56 % from 2020 to 2050 (Fig. 4). The largest reduction (56 %) is from PVAMEMA produced in Estonia in 2050. In 2035 and 2050, PIMA produced in Europe, Norway, or Estonia can mitigate GHG emissions when compared to any fossil counterpart (Fig. 4a). However, PVAMEMA still presents slightly higher climate change impact than PS, in 2035 they are 1.1 to 3.1 kg CO_2-eq./kg polymer higher and in 2050 only 0.4–0.6 kg CO_2-eq./kg polymer higher than PS (Fig. 4b). Furfural-derived UPR production are reduced by up to 47 % in 2050 and reaches similar results to the fossil-based UPR (Fig. 4c).

Implementation of country-specific characteristics (i.e., electricity mixes, biomass composition and transportation distances) has a clear effect on the results. Compared to EU results in 2020, PIMA impacts are 10 % smaller when produced in Norway, and 14 % higher when produced in Estonia in 2020 (Fig. 4a). The life-cycle climate impacts of PVAMEMA are the most affected mostly because of the electricity-intensive depolymerization of lignin. In 2020, when produced in Norway, PVAMEMA results are up to 15 % smaller than the EU average, while in Estonia they are 26 % higher than the EU (Fig. 4b). The furfural-derived UPR production process is the least affected by the country-specific electricity mix (2 %), primarily due to its low electricity demand. The slight variations observed can be attributed to the variations in the forest residue composition across different locations (Fig. 4c).

The uncertainty analysis shows the confidence of the results and robustness of the proposed combined framework to assess emerging bio-based technologies (see Supplementary Table S13 for an overview of the uncertainty sources and corresponding ranges considered in the Monte-Carlo Analysis). The uncertainty ranges of the bio-based impacts are in some cases relatively large, especially for PVAMEMA. This is mainly due to a lower overall yield compared to the other bio-based polymers. For some options, the higher end of the impact is larger than the fossil-based alternative. This indicates the level of improvement that is expected for the bio-based technologies to outperform fossil-based chemicals, and the importance to increase the confidence in the upscaling approaches so that the best performances are implemented. Overall, most of the parameters and assumptions taken in our scaling-up of conversion processes are rather conservative, so the potential impacts of the bio-based polymers at higher TRL are expected to be lower than the fossil alternative, when a full life-cycle and end-of-life perspective are considered.

3.3. Other environmental impacts

The environmental impacts of isosorbide-derived PIMA and vanillin-derived PVAMEMA are compared against their fossil equivalents in Fig. 5, and furfural-derived UPR is compared against fossil UPR in
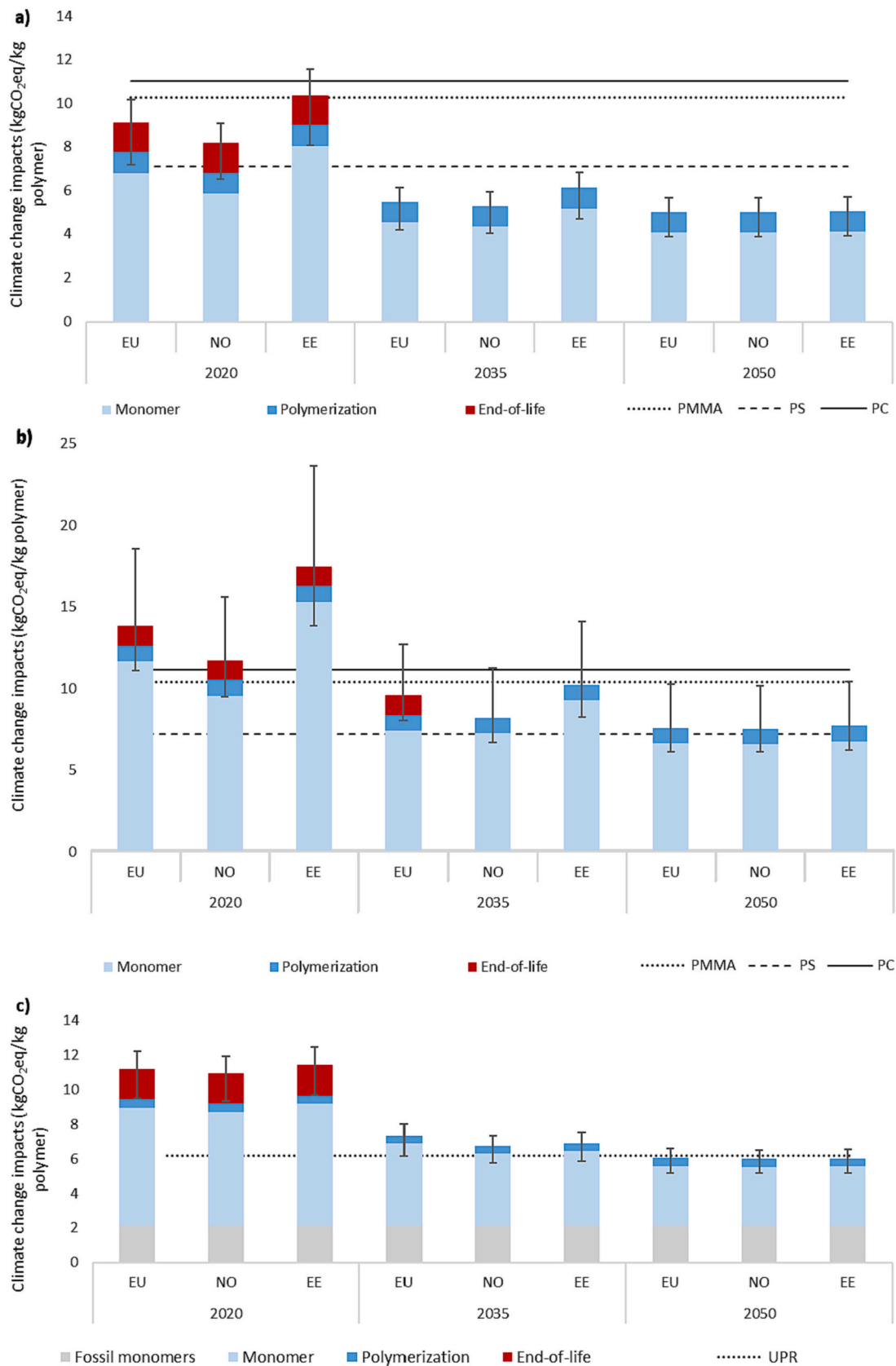
Fig. 4. Impacts of prospective LCA on isosorbide-derived PIMA; b) vanillin-derived PVAMEMA; c) furfural-derived UPR, compared to their fossil alternatives, considering the implementation of SSP2-NDC in Norway, Estonia, and Europe. The biorefinery data used for the analysis are those scaled-up to an industrial level (ex-ante). Uncertainty ranges refer to the results of a Monte Carlo analysis, where lines show the minimum and maximum values.
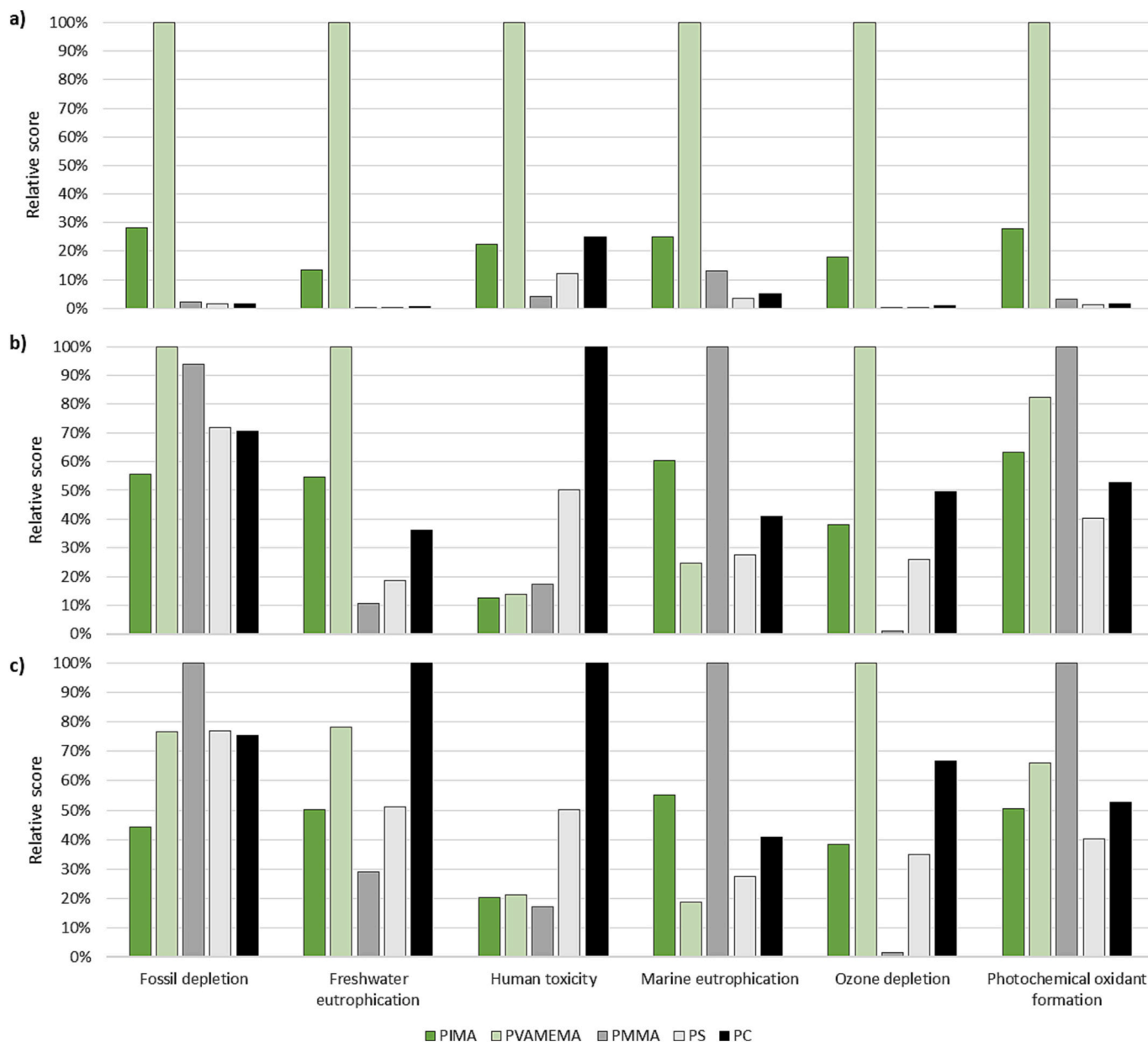

Fig. 5. Environmental impacts of isosorbide-based PIMA and vanillin-based PVAMEMA against their fossil counterparts (PMMA, PS, and PC). Results are shown relative to the worst performance for lab-scale results (a); ex-ante LCA results (b); and combined ex-ante and prospective LCA results (c). Prospective results consider the year 2050 with EU energy mix. Absolute values are available in Table S19.

Fig. S4. For each impact category, results are normalized relative to the highest score and shown for each main phase of the framework, e.g., lab-scale (Fig. 5a), ex-ante LCA (Fig. 5b), and combined ex-ante and prospective LCA (Fig. 5c).

Generally, the results at the lab-scale are higher for the bio-based polymers than the fossil-based polymers, similar to what was observed for the climate change impact in Fig. 3. PVAMEMA shows poor performances in all six categories (Fig. 5a), mostly because of the use of ethyl acetate and methacrylic acid and the relatively high electricity requirements to depolymerize lignin into vanillin. The application of ex-ante LCA improves the bio-based results compared to the ones at lab-scale (Fig. 5b). Identifying and implementing process synergies (e.g., recovery of ethyl acetate and other chemicals) and valorization of side streams notably improve PIMA and PVAMEMA performances in human toxicity, where PC has the highest impacts, and in marine eutrophication and photochemical oxidant formation, where PMMA has the highest impacts. After combining the prospective LCA to the ex-ante LCA

(Fig. 5c), PIMA shows lower impacts than PC, which has the worst environmental performance among the fossil polymers, except for marine eutrophication. This issue can be mitigated by reusing the enzymes, which are the main drivers of impacts in this category. Likewise, the performance of PVAMEMA improves for all impacts except ozone depletion. This impact can be decreased by reducing the use of ethyl acetate and sodium hydroxide. Improvements in the background economy, particularly regarding heat and electricity, are responsible for reducing PVAMEMA impacts on freshwater eutrophication, where PC has the highest impacts, and on photochemical oxidant formation, where PMMA has the highest impacts. While the prospective LCA enhances climate change mitigation, it causes trade-offs with human toxicity. Specifically, PIMA and PVAMEMA show higher impacts in this category compared to their ex-ante LCA results. This decline in performance is attributed to the future electricity mix which contribute to increased human toxicity of the production of chemicals used in the process, namely methacrylic acid and ethyl acetate.

As observed for climate change, even after the application of the combined framework there are bio-based alternatives that do not perform better than the fossil counterparts in some categories. PVA-MEMA still show higher impacts than PC on fossil depletion, ozone depletion and photochemical oxidant formation. There are options that can be implemented to decrease these impacts further, for example optimizing the use of ethyl acetate and methacrylic acid and aim for their replacement with bio-based alternatives (or same chemicals produced from biomass resources). The situation is different when bio-based alternatives are compared to the fossil polymer PMMA, which has higher impacts for climate change, fossil depletion, marine eutrophication, and photochemical oxidant formation, but lower impacts for freshwater eutrophication, human toxicity, and ozone depletion. To outperform PMMA, the production of PIMA and PVAMEMA requires more efficient use of energy and auxiliary chemicals (e.g., ethyl acetate and methacrylic acid), including more efficient depolymerization of lignin into vanillin (for PVAMEMA) and reuse of the methacrylic acid inputs (for both bio-based polymers). The largest challenge is the comparison against PS, as this fossil-based polymer delivered the best environmental performance among the three fossil counterparts. To outperform PS, PIMA requires improvements on marine eutrophication and photochemical oxidant formation, and in a second instance in freshwater eutrophication and ozone depletion, whose impacts are relatively close. More extensive improvements are expected from production of PVAMEMA to reduce impacts relative to PS, as it needs to considerably reduce its impacts for freshwater eutrophication, ozone depletion and photochemical formation. The same improvements mentioned above to outperform PMMA and PC can deliver a better performance of PIMA and PVAMEMA against PS.

In the case of furfural-derived UPR, at a lab-scale this polymer already delivers lower freshwater eutrophication, marine eutrophication, and ozone depletion impacts than the fossil alternative (Fig. S4a). From the fossil monomers that compose UPR, only MA is replaced by a bio-based alternative in this study. Fossil-based MA represents up to 43 % of the UPR impacts in the above-mentioned categories and replacing it with furfural-derived MA led to the better environmental performance. If all the other fossil monomers in UPR are similarly replaced with bio-based alternatives, it has the potential to significantly improve the overall environmental performance. In the ex-ante LCA, identifying process synergies, such as the recovery of acetic acid and catalyst reuse (Fig. S4b), reduced the gap for human toxicity but it is not enough to become better than fossil UPR. As already observed for PIMA and PVAMEMA, the prospective LCA (Fig. S4c) increases impacts in human toxicity, due to future changes in the heat production from wood.

4. Discussion

4.1. Advantages of the combined framework

Integrating ex-ante and prospective LCA, as proposed here, contributes to the need of better methods to assess the environmental impacts of emerging bio-based technologies. The lack of proper assessment methods hinders fair comparison with commercial counterparts and can lead to suboptimal decisions about the deployment of alternative technologies, because the potential environmental benefits that bio-based products could provide are to be assessed at higher maturity levels and in a future economic setting. The currently dominating industrial production of chemicals and plastics has been optimized for decades, reaching very high yields and efficiencies. These and other factors, including low feedstock and process costs, and high feedstock availability (i.e., petrol), challenge bio-based alternatives to compete economically and environmentally with the conventional sector. Unlike to fossil refineries, biorefineries can face challenges like biomass availability and location, seasonality, variability, sustainability aspects connected to previous or alternative land use, and water availability. Producing bio-based chemicals from lignocellulosic residues could help

alleviating part of these challenges. Still, there are risks of resource competition as the same feedstock is attractive for other industries aiming at climate change mitigation, such as the transport sector (especially aviation and shipping) or the metallurgical and cement sectors (where biomass is the main alternative to the use of coal).

In addition to these challenges, unlike heat and energy, that can be produced from resources other than biomass, the options for chemicals and polymers are limited. The sector already faces challenges to achieve carbon neutrality, and this will be amplified in the future as plastics demands are expected to double by 2050 (Stegmann et al., 2022). Currently, only 2.3 % of plastics are bio-based (PlasticsEurope, 2022). There are successful cases of bio-based plastics performing equally or better than fossil counterparts and with great potential to mitigate GHG emissions, as the case of bio-polyethylene (PE) (Brasken, n.d.) and polylactic acid (PLA) (TotalEnergies, n.d.). However, for many applications there are still no viable commercial bio-based alternatives, or they are at very early development stages, showing there is a long road ahead before their successful commercialization. For the latter, developing harmonized methods for ex-ante and prospective LCA that can anticipate potential environmental benefits and trade-offs are key to facilitate sustainability-driven innovation and for a transition of the chemical sector towards an efficient circular bioeconomy.

The combined framework proposed here is a first attempt to provide a consistent environmental impact analysis of emerging bio-based technologies in comparison with their commercial equivalents, so to help to better quantify decarbonization potentials from large scale bio-based chemicals production. The application to a case study shows how the approach can be performed and the relevance it might have for the final outcomes. Performing a conventional LCA of the case study above without the ex-ante and prospective LCA produces results that are up to 43 times higher for climate change impact than their fossil counterparts, which would definitely discourage further research and development investments. Two important contributions of this framework are that it shows that it can be also applied to technologies that are still at a lab-scale with little available data of their potential industrial performance, and that it is easily applicable by LCA practitioners following the proposed step-wise approach, as there is no need for detailed process simulation to arrive at preliminary estimates of environmental impacts if a close dialogue with the chemical experts that performed the laboratory experiments is in place. The stepwise approach makes a distinction between the environmental effects from expected maturity improvements (ex-ante) and from the improvements in the background economy (prospective) that happen outside the system boundaries. Contributions from ex-ante and prospective LCA can thus be isolated, and the potential environmental hotspots can be identified more easily (e.g., the recovery of the solvents in the case study). Scaling-up factors and learning curves can provide meaningful insights but can miss possible bottlenecks and hotspots from aggregating processes, whose identification is instead facilitated by a systematic consideration of each main step and reagent, as in the framework proposed here.

We recommend LCA practitioners to carefully consider four key points when applying the combined assessment framework to emerging bio-based technologies: I) potential reuse of inputs (i.e., chemical and materials), II) potential co-products, III) overall energy requirements, and IV) dialogue with technological experts. At lab-scale, reusing or recovering chemicals and materials is not a common practice, but when processes are implemented at larger scales, it can lead to high environmental impacts, as observed in the case study. As for identifying co-products, the targeted chemical is not always the main or only product of the system. The valorization of side-streams can considerably improve the overall environmental benefits of the emerging bio-based products. In general, energy requirements are not accounted at low TRL, but they can become an environmental hotspot (if not a barrier) for the large-scale implementation of the technology. In order to optimize upscaling projections of system inventories and mass and energy balances for

ex-ante LCA, the LCA practitioners should take decisions in close dialogue with the process developers, here intended as the chemical and/or biochemical experts that conducted the lab or pilot experiments. When this is not possible, they should look for validation of their assumption and projections of industrial scale operations with other experts in chemical engineering, industrial system designing, or process simulation software. This will ensure that the decisions made are feasible and achievable in practice. A clear example from the case study above is the recovery of the main solvents used for both PIMA and PVAMEMA production. This has been considered in the ex-ante LCA thanks to the inputs of the chemical experts that conducted the laboratory experiments in the lab, which confirmed that the solvents can be easily recovered as they are not azeotropic and they are not contaminated during the various reaction mechanisms.

4.2. Limitations of the combined framework

There is still room for improvements for the combined framework proposed here, and they are primarily connected to how ex-ante or prospective LCA are implemented. The prospective LCA reduces indirect emissions from required background chemicals and materials, but most of the reactants are still fossil-based. Changing fossil fuels to renewable feedstocks is expected to provide larger reductions in GHG emissions. The assessed bio-based polymers could also provide other environmental benefits, such as lower toxicity (Ismagilova et al., 2023), but a robust comparison is challenging owing to a lack of data (Fantke et al., 2021) and more tests and experiments are needed.

Process-based calculations, as applied here, are representative of a preliminary process overview, relatively low demanding in time and expertise (Parvakter and Eckelman, 2019), and are widely applied for ex-ante LCA (Tsoy et al., 2020), but they can lose accuracy compared to process simulations. The assumptions for the ex-ante LCA can carry technical simplifications, such as an underestimation of the processes requiring electricity as energy use in pumping of industrial streams or in-belt factory transport of materials that are difficult to estimate beforehand. However, electricity consumption represents, in average, 9 % of the total impact in our case study, and it is unlikely that consideration of consumption from auxiliary processes would significantly change this contribution. Specifically for our biorefinery case study, extra conversion steps might be necessary to make cellulose and hemicellulose sugars available, and depolymerizing lignin efficiently into targeted chemicals needs further development (Kumar and Verma, 2021). Vanillin yield from lignin is still very low and can vary depending on the lignin origin and process applied (Corona et al., 2018; Kumar and Verma, 2021). Today, commercial isosorbide production comes from starch derived from food crops (Roquette, 2020), calling for research and development for its production from lignocellulosic biomass and residues to decrease the potential competition with food.

Finally, there are sustainability aspects that cannot be solved by the combined framework, such as the availability of biomass for the chemical sector. The available existing studies quantify up to 140 EJ of biomass needed to meet both energy and feedstock demands for the chemical sector in 2050 (OECD/IEA, 2018). For the plastic sector alone, estimates of feedstock demand range from 3 to 6 EJ (Stegmann et al., 2022) up to 19–43 EJ (Meys et al., 2021). By means of comparison, the current bioenergy demand is 41 EJ (excluding traditional use of biomass) (IEA, 2023). However, most of the feedstock for chemicals and plastics still comes from food crops and first-generation biomass, and the potential of lignocellulosic residues and second-generation crops has remained constrained. More research and discussion are needed to determine if and what type of chemicals should be produced from biomass. We propose a critical reflection on whether bio-based options are always the best solution for climate change mitigation and what can be sustainably achieved in the chemical sector. Although other sectors are more dependent on fossil fuels and have much higher GHG emissions, the chemical sector is the third largest GHG emitter in Europe (EC,

2023) and the carbon (currently fossil) is not only demanded as an energy source but also as a feedstock (EC, 2023). However, due to the relatively low environmental burden from crude oil extraction and processing associated with naphtha and gas (precursors of most of the chemicals) (OECD/IEA, 2018), some chemicals, such as fossil PS, have efficient and low impact production routes. Even when considering the combined framework, not all bio-based alternatives performed better than their fossil counterpart.

If we manage the end-of-life of PS-based products efficiently, e.g., by improving the waste management, increasing recycling rates and considering incineration with carbon capture and storage or use, their climate impacts can be largely reduced. A comprise to acknowledge limited biomass availability and high efficiency in producing fossil chemicals is to elaborate a strategy where, instead of biomass, fossil carbon is used to produce selected chemicals (e.g., PS, in this case study) that have challenges to be sustainably produced from bio-based sources, as its production is inefficient because of limited maximum theoretical yields or energy intensive treatments or reactants. For these selected challenging-to-be-replaced chemicals, the focus should be shifted from finding alternative sources (i.e., biomass) to developing more efficient end-of-life strategies. This would alleviate resource competition and favor the production of bio-based chemicals that can be produced at higher efficiency (e.g., isosorbide-derived PIMA) and with better sustainability outcomes. Of course, a thorough assessment must consider the whole life-cycle of the products, local biomass constraints, regional specificities (e.g., energy mix, biomass availability, land use conditions, existing infrastructure) and environmental impacts other than climate change.

5. Conclusions

Our analysis proposes a method for integrating ex-ante and prospective LCA for a more robust comparison of the environmental performance of emerging bio-based technologies against fossil-based alternatives. The method is applied to assess the environmental impacts of a case study where novel bio-based polymers from forest residues, that target more demanding application areas, are being developed.

The application of the integrated framework was tested to a biorefinery case study that is still at an early stage of maturity (lab-scale), where the implementation of ex-ante and prospective LCA is exemplified following a stepwise method. In this case, ex-ante LCA reduces climate change impact by up to 98 %, and the major steps that contribute to improving the LCA results relative to the initial lab-scale data are the recovery and reuse of the main solvent, which resulted in up to 83 % reduction of GHG impacts. Ambitious recovery rates and high overall yields considered (i.e., 97 % and 100 %, respectively) are needed for the bio-based polymers to match or outperform conventional fossil alternatives. However, most of the other assumptions taken are conservative and at higher TRL the bio-based polymers are expected to perform better than the fossil alternative, especially when prospective LCA is included. The progressive future developments (e.g., energy decarbonization) in the prospective LCA reduces the climate change impact of the bio-based options by about 56 % by 2050, relative to ex-ante LCA results only, and with the consideration that all the carbon content of bio-based chemicals used as reactants is biogenic the benefits for most of the bio-based chemicals become more evident. Most of the considered chemicals show better climate change mitigation compared to fossil polymers, except for PVAMEMA compared to PS.

Beyond climate change, the application of ex-ante and prospective LCA generally reduces the environmental impacts of bio-based polymers, and isosorbide-based PIMA is a promising potential replacement of PC. However, more improvements are necessary for the other bio-based polymers to robustly outperform the other fossil alternatives.

The combined framework proposed in this analysis clearly separates ex-ante and prospective LCA and introduces a step-by-step approach for the assessment of early-stage bio-based technology. It is a method to

transparently analyses how much production processes at industrial scales can improve relative to lab-scale conditions, and it offers a more robust basis for their comparison with existing fossil-based alternatives. Ultimately, it is instrumental to anticipate potential environmental benefits and trade-offs of emerging bio-based technologies before their introduction to the market, so giving information on systems can be optimized from a sustainability point of view and for which strategic technologies is more relevant to prioritize R&D investments. As this is one of the possible options for defining and integrating ex-ante and prospective LCA, the framework remains open to further improvements by the broader LCA stakeholder community with the aim to achieve consensus for a future common approach. This is particularly relevant as biomass is a limited resource and timely actions are needed to mitigate climate change, and not always bio-based chemicals will deliver better results than the fossil counterparts. LCA practitioners should expand their consideration of integrating ex-ante and prospective LCA to identify those bio-based options that secure the highest environmental benefits, thereby helping to guide research and investments.

CRediT authorship contribution statement

N.R.D. Souza: Conceptualization; Formal analysis; Investigation; Methodology; Visualization; Roles/Writing - original draft; and Writing - review & editing. **L. Matt:** Investigation; Writing - review & editing; **R. Sedrik:** Investigation; Writing - review & editing; **L. Vares:** Funding acquisition; Writing - review & editing; **F. Cherubini:** Conceptualization; Methodology; Supervision; Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.spc.2023.11.002.

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