HEMIC-OAT

Conversion of hemicellulose to coatings

36th CORNET call

D1.4
Interim report on definitions, settings, and system for LCA
(Life Cycle Assessment)

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Collective Research Networking

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Disclaimer

This deliverable has been prepared in the context of the funded project HemiCoat in the framework of the Collective Research Networking (Cornet) supported by the Federal Ministry for Economic Affairs and Climate Action (BMWK, funding code 01IF00399C) through the AiF (German Federation of Industrial Research Associations e.V.) based on a decision taken by the German Bundestag and by the Walloon region as funding with the n° 2310168 (Convention number).

The views expressed in this HemiCoat Deliverable *D1.4 Interim report on definitions, settings, and system for LCA*, which defines the initial methodological framework for the HemiCoat Life Cycle Assessment (LCA) are the sole responsibility of the author and do not necessarily reflect the views of the industries of the User Committee. The User Committee is not responsible for any use that may be made of the information contained therein. The author does not accept any liability for any direct or indirect damage resulting from the use of this Deliverable to its content or parts of it. The results achieved, conclusions made, and recommendations given by the author should not be interpreted as a political or legal signal that the European Commission or any other political or legal institution intends to take a given action.

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Abbreviations

Abbreviation	Description
EF	Environmental Footprint (Life Cycle Impact Assessment Methodology)
FU	Functional Unit
HC	Hemicellulose
IA	Itaconic acid
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MCS	Monte Carlo Simulation
PAA	Polyacrylic acid
PIA	Polyitaconic acid
SDS	Sodium dodecyl sulfate
SME(s)	Small and medium-sized enterprise(s)
UC	User Committee
WP	Work package
Unit abbreviation	
CTU_e	Comparative Toxic Unit for the ecosystem
CTU_h	Comparative Toxic Unit for human
kBq U^{235}	kilobecquerel of $Uranium^{235}$
kg CFC-11 eq	kilogram of CFC-11 (Trichlorofluoromethane) equivalent
kg CO_2 eq	kilogram of carbon dioxide equivalent
kg N eq	kilogram of nitrogen equivalent
kg NMVOC eq	kilogram of non-methane volatile organic compounds equivalent
kg P eq	kilogram of phosphor equivalent
mol H^+ eq	mole of hydrogen ion equivalent
mol N eq	mole of nitrogen equivalent
kg world eq. deprived	equivalent kilogram of an average global resource made unavailable
kg Sb eq	kilogram of antimony equivalent

1. Executive summary

Deliverable *D1.4 Interim report on definitions, settings, and system for LCA (Life Cycle Assessment)* is the relevant preparatory work for *D1.5 LCA of hemicellulose oligomers and itaconic acid-based products* in the HemiCoat project by providing the initial definitions, and settings, including the goal and scope definition and system descriptions, as well as all relevant technological parameters for the further tasks integrated in *D1.5*. Therefore, this report is essential to Work package *WP 1 Biomass Potential & Life Cycle Assessment*, which is under the responsibility of DECHEMA e.V. and DBFZ gGmbH. The present deliverable is based on the exchanges during the 1st HemiCoat meeting, 28.10.2024, at DBFZ gGmbH in Leipzig (Germany), and the 2nd HemiCoat meeting, 16.04.2025, at Celabor s.r.l. in Chaineux (Belgium), as well as the consortium's monthly online meetings. This consortium consists of the following partners: DECHEMA e.V., DBFZ gGmbH in Germany, Celabor s.r.l., Materia Nova in the Walloon region.

2. Introduction

HemiCoat's overall project objective is to valorize hemicellulose (HC) by-products from paper pulp manufacturing and agricultural lignocellulosic biomass to obtain added-value products. Herein, the project represents the idea of utilizing all components of natural commodities, specifically of wood, to maximize resource efficiency, reduce waste, and improve the sustainability of biomass utilization. Woody biomass offers unique properties that can be valorized into high-value products, contributing to a circular (bio-)economy. This holistic approach can minimize environmental impact, lower fossil resource dependency, and enhance the economic viability of wood-processing industries. However, HC, a significant fraction of the woody biomass, remains largely underutilized despite its potential to produce bio-based, sustainable alternatives to fossil-derived products. It is used mainly to recover energy through burning. Simultaneously, the coatings and adhesives industries are facing increasing demand for bio-based, low-carbon products that reduce reliance on fossil resources, align with regulatory changes, and eliminate hazardous compounds.

The HemiCoat (Hemicellulose to coatings) project aims to valorize HC streams, particularly HC breakdown products obtained from isolation processes for cellulose and lignin, to produce added-value chemicals for coatings, adhesives, and functional additives. HC monomeric pentoses are fermented into itaconic acid (IA), which undergoes further chemical modifications. In a parallel approach, HC oligomers are transformed chemically into sustainable wood adhesives. **Figure 1** shows an overview of the HemiCoat processes.

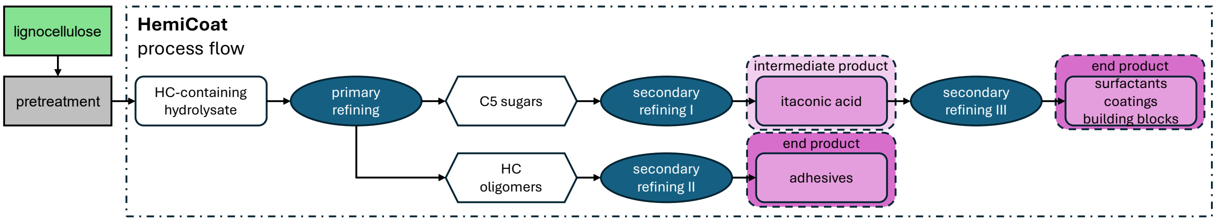

Figure 1. Overview of the HemiCoat process flows.

HC breakdown products from differently pretreated wood hydrolysates are separated in a primary refining process to obtain a C5 sugar (pentose) fraction, mainly xylose, and HC oligomers. In secondary refining, the xylose is fermented to IA, the key intermediate product chemically modified in a secondary refining III to produce surfactants or coatings, the end products of the HemiCoat process flow. In a parallel process, HC oligomers, after primary refining, are transformed into adhesives in secondary refining II. The resulting adhesives are the second line of end products of the HemiCoat process.

To investigate if the HemiCoat concept minimizes the environmental impact compared to traditional methods for producing surfactants, coatings, and adhesives from fossil sources, an attributional Life Cycle Assessment (LCA) will be performed. At a later stage of the project, the environmental impact of the production of IA using the process developed in HemiCoat will be investigated and compared to the production of IA from wheat straw.[1] Therefore, this report (*D1.4 Interim report on definitions, settings, and system for LCA*) aims to prepare the evaluation of the potential sustainability benefits of the innovative HemiCoat processes to allow the comparison of the intermediate(s) and final product(s) with conventional/fossil equivalents. Herein, this report defines the initial methodological framework of the attributional LCA to evaluate the sustainability and environmental impact of the HemiCoat process chains, which is designed to

[1] Rebolledo-Leiva, Moreira, and González-García, "Environmental Assessment of the Production of Itaconic Acid from Wheat Straw under a Biorefinery Approach."

align with the needs of small and medium-sized enterprises (SMEs) in Europe. The LCA (*D1.5 LCA of hemicellulose oligomers and itaconic acid-based products*), which is the follow-up of this report, will comprehensively assess the environmental performance of these innovative processes while identifying potential trade-offs and areas for improvement.

2.1. Mapping HemiCoat's outputs

This section aims to map HemiCoat's grant agreement commitments within the formal deliverables and task descriptions against the project's respective outputs and work performed. This report is listed as Deliverable *D1.4 Interim report on definitions, settings, and system for LCA* and is due in M9 of the project, June 2025, representing the preparatory work for *D1.5 LCA of hemicellulose oligomers and itaconic acid-based products*, which is due in M24, August 2026. Both deliverables are assembled in *WP 1*, *task 1.4 Life Cycle Assessment*. **Table 1** lists, describes, and justifies the tasks and subtasks in HemiCoat connected to the report.

Table 1. Adherence to HemiCoat's task description & Deliverables.

<table>
<tr><th>HemiCoat task</th><th>Description</th><th>Justification</th></tr>
<tr><td>Task 1.4 Life Cycle Assessment (M4 to M24)</td><td>Results from experimental work, feedstock potential analysis, and market analysis will be used to conduct an LCA of the entire process chain, which leads to D1.5 LCA of hemicellulose oligomers and itaconic acid-based products.</td><td>Evaluation of the environmental impacts of products and processes across the HemiCoat production chain, enabling sustainability improvements</td></tr>
<tr><td>Subtask 1.4.1 Definitions and settings</td><td>Identification of crucial parameters of the LCA</td><td rowspan="2">Provides the basis for task 1.4 in WP 1, allows for consistent results, and enables appropriate data collection for the other tasks involved in WP 1.</td></tr>
<tr><td>Subtask 1.4.2 Qualitative system description</td><td>Definition of the system boundaries, key processes, and interactions within the product life cycle without using quantitative data, providing an overview of inputs, outputs, and environmental considerations.</td></tr>
<tr><th colspan="3">HemiCoat Deliverables</th></tr>
<tr><td colspan="3">D1.4 Interim report on definitions, settings, and system for LCA.
The report defines the initial methodological framework for the HemiCoat LCA in D1.5.</td></tr>
<tr><td colspan="3">D1.5 LCA of hemicellulose oligomers and itaconic acid-based products.</td></tr>
</table>

The HemiCoat LCA interim report *D1.4*, defining and setting up the LCA system, will pave the way for the attributional LCA at a later stage of the project, which will quantify the environmental impact of utilizing HC streams in the scope of the project, offering an understanding of whether bio-based products from HC side streams may contribute to sustainability goals. An economic analysis of the HemiCoat process cascade is performed in Deliverable *D1.6 HemiCoat market analysis and exploitation strategy* and thus is excluded from this report. However, ecological and economic analyses are combined and form the sustainability assessment in HemiCoat.

2.2. Sustainability assessment in HemiCoat

The sustainability assessment within HemiCoat is integrated in the work package 1 (*WP 1 Biomass potential & Life Cycle Analysis*), whose main objectives include:

- The assessment and improvement of the sustainability impacts of the HemiCoat processes and products by providing objective information regarding key sustainability aspects using scientific, transparent, and reproducible methodologies.

- The assessment of the sustainability and techno-economic feasibility of the HemiCoat processes and products, along with their production in a comprehensive manner. Herein, the process assessment will be based on the technical results of *WP 2 to WP 4* and, if required, supplemented by literature.
- The provision of iterative feedback to the process developers as part of *WP 2, WP 3,* and *WP 4* to further optimize the processes in the form of estimation and up-scaling of woody biomass & hydrolysate potential from industry, and an ecological assessment (LCA), as well as an economic evaluation of the HemiCoat products.

The main objective of *WP 1* is to assess the sustainability of the HemiCoat value chains comprehensively, covering two key aspects of sustainability: environment and economy. **Figure 2** maps *D1.4 Interim report on definitions, settings, and system for LCA* within the Sustainability Assessment in *WP 1* and interconnects the *WP*s (see section *2.1 Mapping HemiCoat's outputs*).

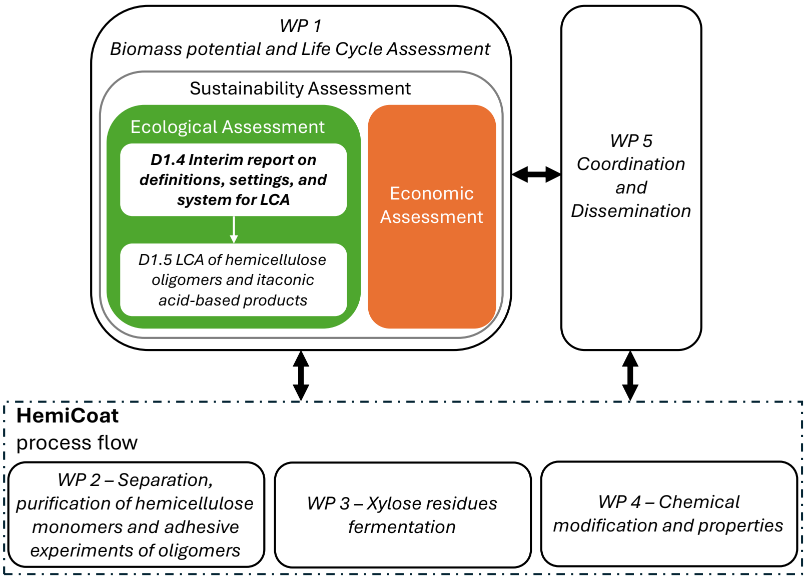

Figure 2. Work packages in HemiCoat and mapping of the present report within the sustainability assessment.

The social dimension is excluded from the investigation since it is not among the main drivers of sustainability in this context, being considered indirectly through existing corporate policies. The comparable small relevance of social aspects in the HemiCoat concept can be explained in the following:

- Well-established regulatory and social standards exist in Central and Western European industries, such as Germany and Belgium – the regions of the project – due to strict labor laws, workplace safety regulations, and social responsibility requirements enforced by the EU and national governments.
- The overall minimal direct social impact in highly automated processes in industries connected to the HemiCoat processes, which often rely on specialized labor (and automatization), and thus fewer human workers are directly affected by daily operations.

On the other hand, economic and environmental aspects, with their quantifiable metrics e.g., CO_2 equivalent emissions, resource use, economic growth, etc. are prioritized in HemiCoat's sustainability assessment, since both, economic viability and environmental compliance, are required in the competitive industrial sectors connected to HemiCoat (e.g. manufacturing of chemicals and chemical products, reclaimed wood processing, ...) to remain the competitiveness in the European and global market.

The sustainability assessment will reveal the advantages, disadvantages, and trade-offs in the HemiCoat value chains compared to established routes. The HemiCoat value chains are the sequential workflow from the production of the HC hydrolysates to the desired final products and product classes of the project:

1. Separation and purification of HC monomers and adhesive experiments of oligomers (WP 2)
2. Xylose residues fermentation to IA (WP 3)
3. Chemical modification and properties (WP 4)

For reliable and robust sustainability assessment results, the principles of comprehensiveness during the life cycle stages of products must be considered. A systematic overview will allow to identify and possibly minimize the unintentional shifting of environmental burden and economic benefits between life cycle stages or individual processes. The production of IA, the key intermediate product of the HemiCoat process flow, will be compared to alternative production route(s) from literature, e.g., from wheat straw under a biorefinery approach.[2] Likewise, the sustainability performance of HemiCoat end product production(s), e.g., polyitaconic acid (PIA) will be compared to described routes.[3]

The sustainability assessment in HemiCoat evaluates the feasibility to minimize selected environmental impacts, such as emissions or energy demands, compared to a benchmark while maintaining competitive production costs in a commercial-scale setup. This is accomplished by translating experimental data from other project WPs and implementing them into life cycle assessment models. The final integrated assessment(s) will utilize a multi-criteria evaluation software tool, allowing to identify potential optimization pathways for the production of IA and the HemiCoat end products.

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[2] Rebolledo-Leiva, Moreira, and González-García.

[3] Nuss and Gardner, "Attributional Life Cycle Assessment (ALCA) of Polyitaconic Acid Production from Northeast US Softwood Biomass."

3. Definitions and settings for the ecological sustainability assessment

The (ecological) sustainability assessment requires common definitions and settings on which the environmental (and economic) evaluation will be based to ensure consistent data and results.

3.1. The HemiCoat biorefining concept

The HemiCoat project aims to valorize hemicellulose (HC) breakdown products from isolation processes for cellulose and lignin to obtain high value-added chemicals toward sustainable coatings, adhesives, and functionalized additives. The overall goals of the project are:

- Recovery of most of the HC oligomers from lignocellulose biomass processing
- Feasibility tests of the manufacturing of adhesives from the HC oligomers
- Use of the monomeric sugars and other residual compounds in a fermentative step to produce IA
- Usage of IA as a building block for chemical synthesis of surfactants and coatings

The overall concept of the HemiCoat biorefining project can be summarized in a primary refining and three secondary refining steps. In the primary refining, HC oligomers and C5 sugars are recovered and purified from wood-born hydrolysates. In the secondary refining step I, the concentrated and purified monomeric C5 sugars are fermented in a fed-batch process to IA. In parallel, in the secondary refining step II, the hydrolysate-born hemicellulosic oligomers are applied in formulations with chitin/chitosan as wood adhesives. Finally, in a secondary refining step III, the product of the secondary refining step I, IA, is purified for subsequent chemical modification to produce biobased products, e.g., surfactants or coatings. **Figure 3** shows the overall concept of the HemiCoat biorefining concept.

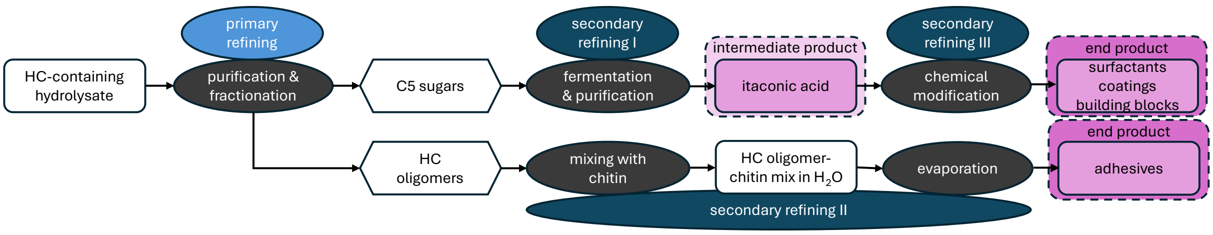

Figure 3. The HemiCoat refining concept.

The overall goal of HemiCoat is to gain a sustainable and cost-effective purification and conversion of sugars from the HC fraction of lignocellulosic biomass to produce bio-renewable surfactants, coatings, and adhesives for applications. This can help SMEs that work with IA-based products by diversifying sources of supply, increasing quality, or decreasing costs. Moreover, HemiCoat may open the possibility of technological breakthroughs for related SMEs, such as the companies represented in the User Committee (UC) of the project, to replace their commonly used fossil-based reagents and materials with bio-based alternatives from IA and extend the field of application toward functionalized additives or coating materials. Likewise, the project can offer the potential to impact SMEs interested in the valorization of (their) lignocellulosic and hemicellulosic agro-industrial wastes and, therefore, can open new and sustainable business perspectives.

3.2. Goal and scope definitions and settings for the LCA

The goal and scope definition phase is a critical first step in an ISO-standardized LCA. In this phase, the purpose of the assessment is established, and key decisions are made regarding the details of the product system under study. According to ISO 14040[4] and 14044[5], this phase is more than just an introduction to the LCA process, but plays a fundamental role in shaping the entire LCA study. Before data collection begins, by defining the goal and scope at the outset, it can be ensured that the methodology is structured and aligned appropriately with the intended objectives, and the foundation for a robust and meaningful LCA is set.[6]

The initial planning phase of the (HemiCoat) LCA study involves defining key aspects such as the study's objective, target audience, and product characteristics – including function, functional unit, and reference flows. Additionally, it establishes essential scope elements, including system boundaries, cut-off criteria, regional coverage, and considerations for multifunctionality.

3.2.1. Goal of the LCA

HemiCoat's attributional LCA aims to identify the implications of project process flows, including all optimizations for the processes.

The primary *aim of the study* is to provide decision support for two main applications:

- the development of sustainable products based on a resource-efficient concept
- an improved technology development in comparison to a non-optimized process flow and to other approaches from literature

The *target audience* of the study is decision-makers in the following fields:

- Research: Academic and research institutions such as universities and research centers contribute expertise in biomass valorisation, LCA methodologies, process optimization, and material characterization
- Industry: SMEs (and large enterprises) being engaged in hemicellulose extraction, chemical modification, and the formulation of bio-based coatings or surfactants.
- Policy, Regulatory and Certification Entities: Compliance with sustainability directives is governed by national and European regulatory bodies, ensuring alignment with environmental and industrial policies.
- General public.

For these key stakeholders and institutional involvement, the following *main guiding question* occurs in HemiCoat's sustainability assessment.

How far and under which conditions can different hydrolysates (containing hemicellulosic sugars as byproducts from the production of cellulose or lignin products) be used according to the HemiCoat process flow and contribute to a sustainable supply of the targeted biobased coating, surfactants and adhesives?

It is the goal of the final sustainability assessment report at the end of the project to answer this question. The main guiding question leads to the following *sub-questions*:

[4] "ISO 14040:2006 Environmental Management — Life Cycle Assessment — Principles and Framework."
[5] "ISO 14044:2006 Environmental Management — Life Cycle Assessment — Requirements and Guidelines."
[6] Curran, "Overview of Goal and Scope Definition in Life Cycle Assessment."

1. How do the HemiCoat process flow cascades compare from a sustainability perspective to the conventional production of:
   1.1. IA
   1.2. Sugar-oligomer-based adhesives (vs. the end products of the secondary refining step II)
   1.3. IA-based surfactants and coatings (vs. the end products of the secondary refining step III)
2. How do specific results from environmental and economic perspectives differ?
3. Which unit processes determine the results most, and what are the optimization potentials?
4. What would the impact of possible economic transitions (e.g., towards renewable energy, intensified usage of HC by-products) be?
5. Which barriers (e.g., technological) and limitations (e.g., biomass availability) may hinder the industrial-scale implementation of the HemiCoat processes or require changes to the concept that affect sustainability?

3.2.2. Scope definition

The scope of an (attributional) LCA study specifies the products and systems to be analyzed. It must be well-defined to ensure that the study's comprehensiveness, depth, and detail align with its stated goal(s) (see 3.2.1). The resulting definitions and parameters guide subsequent analyses, ensuring consistency across environmental assessments. Key scope parameters – including system definitions, functions, and geographical considerations – are outlined in the following sections.

3.2.2.1. System boundaries and modularity of the LCA

The definition of the boundaries is required to outline the investigated product system(s) and its overall function(s). The boundaries selected for the HemiCoat project comprise the Cradle-to-Gate analysis shown in **Figure 4**. To cover all the process flows and to obtain an ecological assessment of the key intermediate product IA, as well as the final products, three LCA modules are designed:

- LCA module 1 – From Hemicellulose to IA
- LCA module 2 – From IA to IA-based coatings, e.g., sulfonated IA-esters, IA-polymers
- LCA module 3 – From Hemicellulose (oligomers) to coatings (oligomeric sugar-chitin/chitosan mixtures)

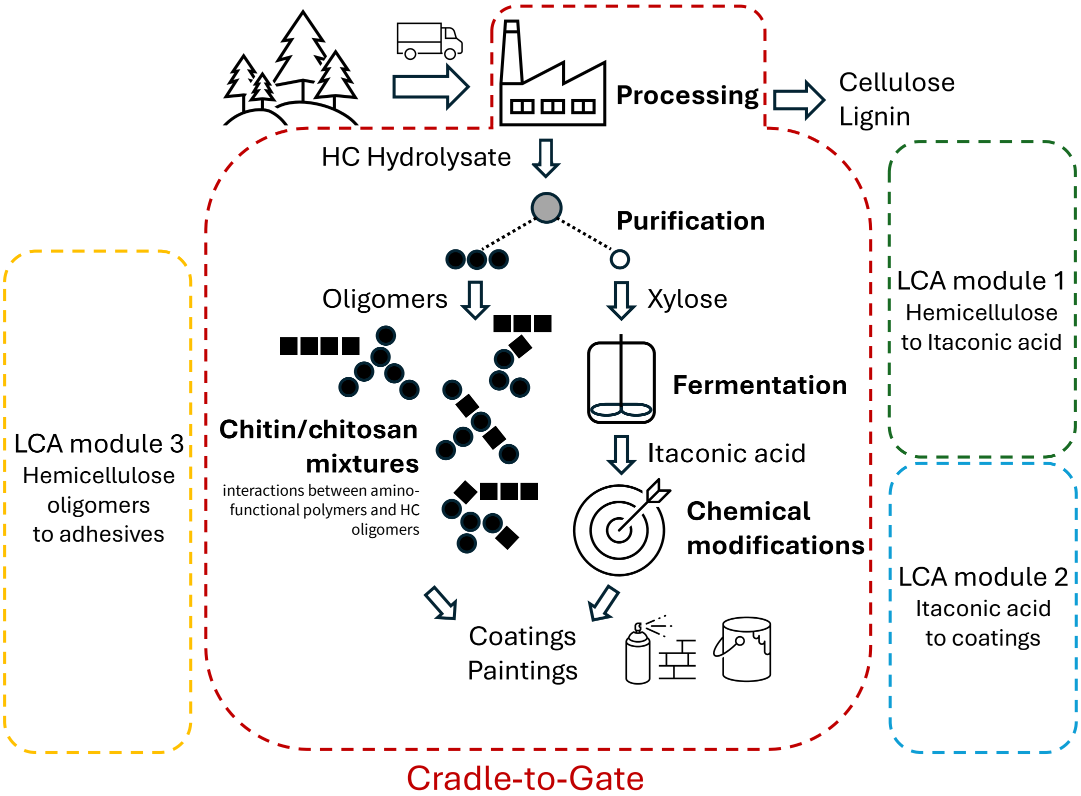

Figure 4. Overview of the system boundaries of the HemiCoat LCA.

The HemiCoat Cradle-to-Gate LCA covers all process flows from wood processing to obtain HC hydrolysates, the purification into sugar oligomers and monomers, and the fermentation of sugar monomers into IA until the production of adhesives, coating, and surfactants by chemical modification of the IA or the purified sugar oligomers. Three LCA modules will be conducted and combined to evaluate the key steps of the HemiCoat process flow ecologically.

The processes and flows of LCA module 1 and LCA module 2 can be directly linked since IA – the product of the process of module 1 – is the input material of the process covered by module 2. Likewise, module 1 and module 3 can be linked since HC oligomers, being another product of module 1, are the input of the process covered by module 3. The detailed depiction of the HemiCoat LCA modules and their interconnection is shown in **Figure 5**, with an overview of the material and energy flows. The combination of the three LCA modules will provide the HemiCoat LCA Cradle-to-Gate analysis and, thus, the ecological assessment of the project.

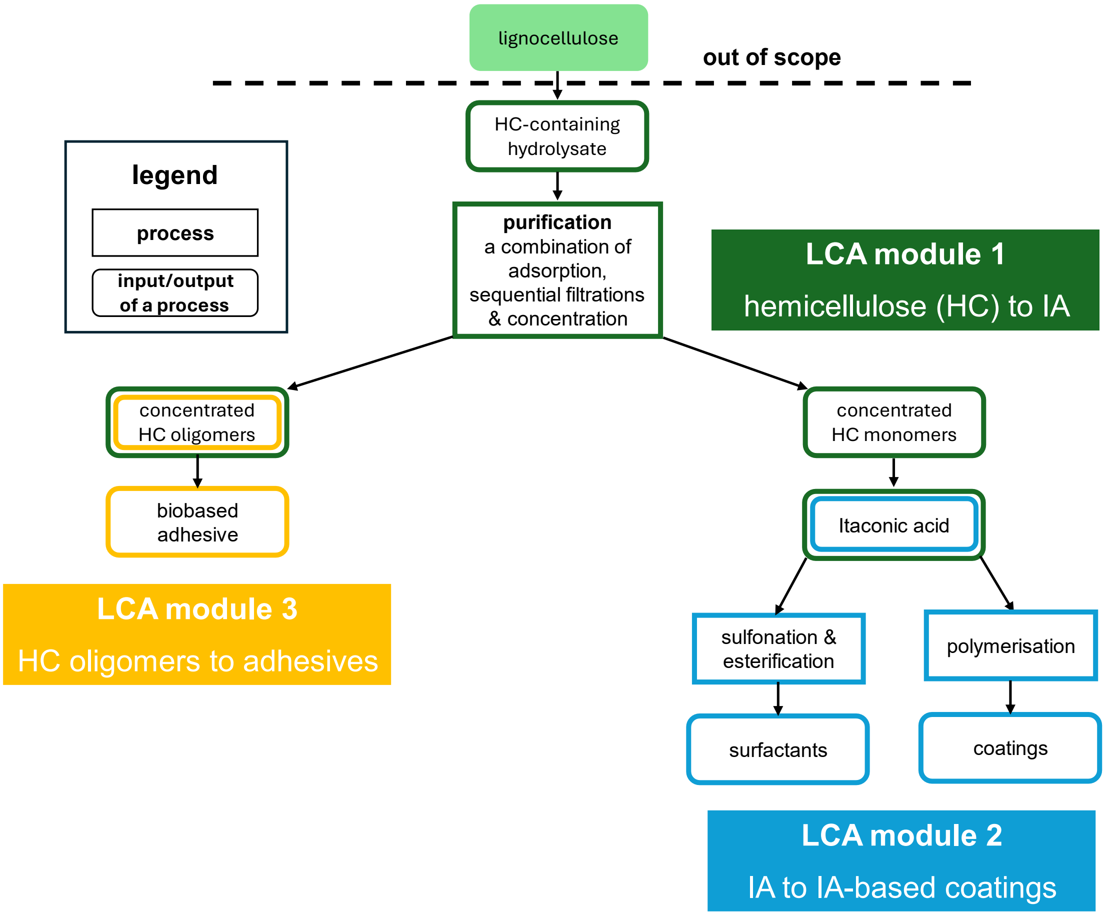

Figure 5. LCA modules within the system boundaries of the HemiCoat LCA.

The three LCA modules are displayed in dark green (module 1), blue (module 2), and orange (module 3). Flows within one module are framed in the respective color, e.g., processes covered by LCA module 1 are framed in green. Both colors of the respective LCA modules frame interconnecting flows (shared intermediates).

3.2.2.2. Functional Unit

Defining a system's function and establishing an appropriate functional unit (FU) are critical components in conducting an (attributional) LCA. The functional unit covers qualitative and quantitative aspects of the system's function by addressing key parameters, e.g., what is being assessed, in what quantity, and in what quality. These elements are fundamental to ensuring a valid comparison between different systems. Noteworthy that the parameter time (duration) will be excluded from the consideration. For a complex process cascade, which operates as a multi-output process generating multiple products, such as in the HemiCoat project, a distinct functional unit must be defined for the product(s) (of the three LCA modules) to enable a meaningful comparative assessment.

For IA, the product of LCA module 1, the FU is defined by 1 kg of IA with a 99 % purity as described in a previous report on the environmental assessment of the production of IA from wheat straw in a biorefinery approach.[7] Likewise, FU of IA-based surfactants, which are various anionic esters of sulfonated IA and alcohols and of IA-polymer coatings (LCA module 3) as well as of HC-oligomer-based adhesives (LCA module 2), are defined by 1 kg product with a 99 % purity.

[7] Rebolledo-Leiva, Moreira, and González-García, "Environmental Assessment of the Production of Itaconic Acid from Wheat Straw under a Biorefinery Approach."

3.2.2.3. Cut-off criteria

Mass and energy thresholds are applied as the cut-off criterion in the attributional HemiCoat LCA. Consequently, the cut-off should be viewed as a data collection threshold, below which further data collection is unnecessary due to negligible contributions.[8] This approach intends to account for the average environmental burden associated with the lab-scale process cascade of the system. By setting a threshold of 1 % of the mass or energy inputs, which is expected to be significantly smaller than the scaling factors within the LCA, minor flows are excluded to streamline the inventory while maintaining the integrity of the results. This is particularly relevant in cascade systems, where the sequential nature of the process can introduce small, iterative inputs that are not representative of industrial-scale operations. The use of mass and energy cut-offs ensures that the assessment remains focused on the most significant contributors. Following the guidelines set in ISO 14044[9] within one LCA module, the cumulative contribution of all excluded inputs will be verified to be below 5 % of the total environmental impact evaluated by the Global Warming Potential (GWP100). In a preliminary screening LCA, the potential impacts of all flows – including those considered for exclusion – will be estimated and compared against the overall system impact across relevant categories such as GWP100 and cumulative energy demand.

3.2.2.4. Geographical coverage and regional factors

The geographical scope of the LCA report (*D1.5 LCA of hemicellulose oligomers and itaconic acid-based products*), which is the follow-up to this report, will cover Germany and Belgium, capturing the entire process chain from raw material treatment to intermediate processing and the formulation of hemicellulose-based coatings, surfactants, and adhesives. This assessment follows the Cradle-to-Gate approach, prioritizing regional biomass utilization, industrial processing emissions, and interregional logistics. Thus, the following regional factors influencing the process chain are identified:

- Feedstock availability and supply chain logistics: The availability of hemicellulose-rich (agro-)industrial by-products in Belgium and Germany dictates sourcing strategies and process feasibility. This is the target of the report *D1.1 Estimation of woody biomass and wood hydrolysate from industry in Belgium and Germany*.
- Infrastructure and transport emissions: The transboundary movement of processed intermediates may contribute to the life cycle impact profile.
- Energy grid variability: Disparities in energy production portfolios between the two nations may influence the carbon footprint of energy-intensive processing steps.

The energy grid variability is displayed in **Figure 6** comparing the share of energy production by source in Germany, Belgium, and the European Union in 2022.

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8 Laurent et al., "Methodological Review and Detailed Guidance for the Life Cycle Interpretation Phase"; Gradin and Björklund, "The Common Understanding of Simplification Approaches in Published LCA Studies—a Review and Mapping."

9 "ISO 14044:2006 Environmental Management — Life Cycle Assessment — Requirements and Guidelines."

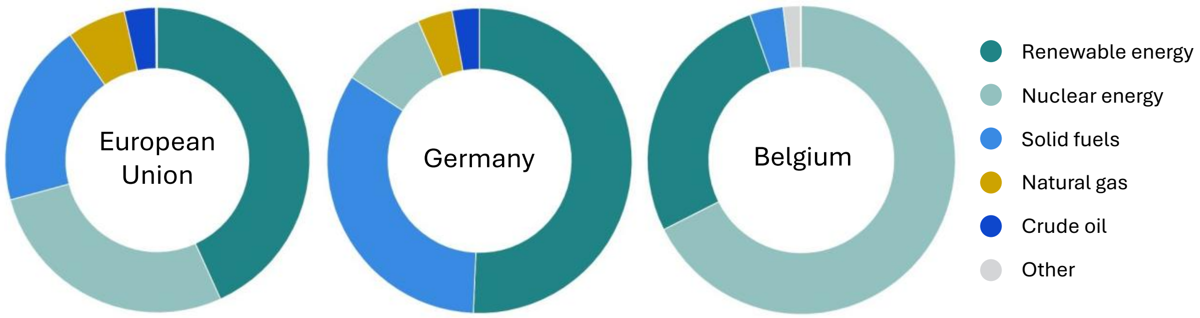

Figure 6. Energy production by share of source in the European Union, Germany, and Belgium in 2022.[10]

When evaluating the geographical scope and regional factors, it is crucial to ensure that the defined boundaries correspond to the study's intended purpose and account for regional differences in environmental impacts. The geographical boundaries define the relevance of data sources, regulatory frameworks, energy mixes, and transportation distances, all of which influence the overall LCA results. Data sources and input considerations for the LCA are analyzed in the next section.

3.3. Data sources and input considerations

3.3.1. Primary data acquisition

Primary data collection is crucial for ensuring an accurate representation of the processes. In this assessment, data is gathered from laboratory-scale processing experimental data from HemiCoat WPs, which provide insights into energy consumption, raw material utilization, process efficiency, and waste generation under controlled and optimized experimental conditions.

3.3.2. Secondary data utilization

Background datasets from reputable sources in Ecoinvent v3.11 and potentially other databases will complement primary data. These databases offer industry-verified life cycle inventory (LCI) data, supporting impact modeling by providing emission factors, energy mix compositions, and material-specific environmental burdens. Existing literature sources, such as peer-reviewed studies and industry reports, provide valuable information on materials, energy use, emissions, and environmental impacts. In this context, a careful selection of reliable and relevant sources is the key to ensuring data quality and maintaining assessment credibility. Additionally, secondary data from the industrial-scale process simulation on the HemiCoat process cascade performed by the DBFZ will provide further inputs. Overall, the integration of secondary data enhances the robustness of the assessment and ensures consistency with established LCA methodologies.

3.4. Life Cycle Inventory (LCI)

The Life Cycle Inventory (LCI) phase systematically quantifies energy and material inputs, emissions, and waste outputs across the HemiCoat process flow and is outlined in this section. Herein, the key processes are discussed and displayed in **Figure 7** as the scheme of the process and energy flows of the HemiCoat LCA (modules).

[10] European Union, "Interactive Publications Shedding Light on Energy in Europe – 2024 Edition."

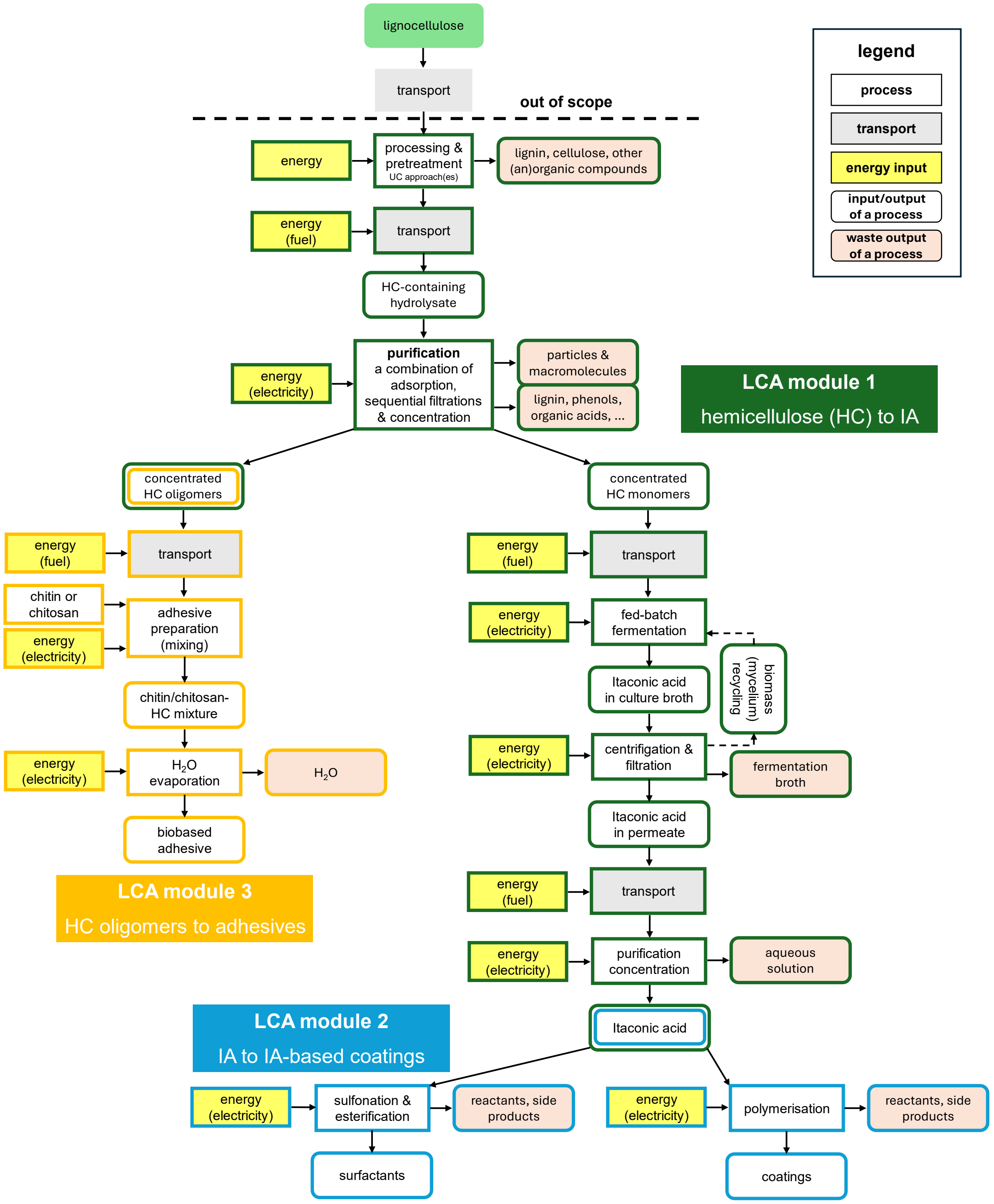

Figure 7. Process and energy flows of the HemiCoat LCA modules

The HemiCoat Cradle-to-Gate LCA, which is composed of LCA modules 1, 2, and 3, covers all process and energy flows from the processing of the hemicellulose-containing woody raw material (lignocellulose) to the production of adhesives, surfactants, and coatings. In the initial stage, the processing and pretreatment method for lignocellulose employed by one or more members of the User Committee (UC) is evaluated.

Figure 7 presents a comprehensive depiction of processes and energy flows within the project and, therefore, is the guideline for the subsequent analysis of HemiCoat LCA. To ensure a systematic and rigorous examination, this section is organized in a framework that facilitates a coherent transition from data representation to interpretation, thereby enabling a comprehensive and scientifically robust assessment of LCA study in the HemiCoat project.

3.4.1. Biomass pretreatment, hemicellulose separation, sugar extraction, and Itaconic acid fermentation

The separation of hemicellulose from biomass and the extraction of sugar mono- and oligomers require an in-depth analysis of:

- Raw material sourcing and processing (based on the approach of at least one member of the UC).
  - The approach will be selected to prioritize fermentation-ready or easy-to-pretreat hydrolysate with minimal downstream conditioning, backed by a life-cycle record and large-scale (ideally ton-scale) availability.
- Energy inputs associated with biomass pretreatment, extraction methods, and the fermentation of IA.
- Chemical consumption and potential emissions from the extraction and the fermentation process.
- Waste streams, including unvalorized biomass fractions and effluents.

The products of these processes are a concentrated hemicellulose-oligomer fraction and IA. This process cascade is analyzed in LCA module 1.

3.4.2. Adhesive formulation and functionalization of Itaconic acid for coatings and surfactants

The production of coatings and surfactants and the formulation of biobased adhesives from the HemiCoat process flow involves multiple chemical processing steps for which the following analysis is considered:

- Optimization of the reaction conditions.
- Energy consumption and emissions from synthesis and purification processes.
- Environmental impacts of solvents, catalysts, and stabilizers (if applied).
- Efficiency of coating application and material utilization rates.

In one approach, the fermented and concentrated IA is chemically converted to surfactants and coatings, which are analyzed in LCA module 2 of the HemiCoat project. In another approach, the concentrated HC-oligomer fraction undergoes a treatment process with chitin and chitosan, respectively, to yield biobased adhesives, which are analyzed in LCA module 3.

3.4.3. Logistical and interregional transport impacts

The transportation of (intermediate) materials and products may contribute to the overall environmental impact. Therefore, the assessment quantifies:

- Fuel consumption and emission factors associated with transportation (e.g., road, rail).
- Supply chain distribution distances and their influence on carbon footprint.
- Packaging materials and their end-of-life disposal implications (if they are within the cut-off criteria defined in 3.2.2.3).

The HemiCoat LCI integrates empirical and secondary data to provide a holistic evaluation of the environmental performance of the HemiCoat processes. By systematically compiling and analyzing LCI data, the study enables informed decision-making for process optimization and sustainability improvements. Future work may involve refining data precision through additional experimental validation and exploring alternative process configurations for impact reduction.

The final integrated assessment(s) will utilize a multi-criteria evaluation software tool, allowing for the comparison of different impact categories and sensitivity analyses to identify potential optimization pathways to produce IA and further HemiCoat end products. The following section addresses the inventory analysis. Herein, primary and secondary data will be integrated to provide a comprehensive and accurate representation of the system's environmental footprint.

3.5. Inventory analysis – Impact assessment methods

For the LCA of the HemiCoat process flows the software tool openLCA[11] will be used. In openLCA, the choice of Life Cycle Impact Assessment (LCIA) method depends on the study's goals, scope, and regional context. Several widely recognized methods are commonly employed, each with distinct advantages. Most applied methods are ReCiPe and Environmental Footprint (EF), which are covering the broadest set of environmental impact categories.

3.5.1. Selection of the LCIA method in openLCA

While the ReCiPe method provides a flexible framework applicable on a global scale, the EF method stands out as the preferred choice for studies within the European context due to its standardization, policy alignment, and enhanced comparability. The EF method ensures consistency across assessments, making it particularly valuable for businesses and organizations aiming to comply with EU sustainability regulations and reporting requirements, such as the recently announced Corporate Sustainability Reporting Directive (CSRD).[12] Therefore, the European Commission recommendation (EU) 2021/2279 aims for the usage of EF to measure and communicate the LCA performance of products (and organizations) as stated in the Official Journal of the European Union L 471, volume 64.[13]

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[11] "OpenLCA."

[12] Operato et al., "Navigating CSRD Reporting: Turning Compliance into Sustainable Development with Science-Based Metrics."

[13] European Union, "Official Journal of the European Union L471."

The EF method provides a reduced variability by using harmonized datasets and sector-specific guidelines, improving the reliability and transparency of results. This level of standardization is essential for benchmarking environmental performance across industries, facilitating clearer decision-making and policy implementation. Consequently, for those prioritizing regulatory compliance, consistency, and sector-specific applicability, the EF method is the superior choice over ReCiPe, particularly in studies that require alignment with European environmental policies and initiatives, such as the HemiCoat project.

3.5.2. Environmental Footprint (EF)

The Environmental Footprint (EF) method is an LCA-based approach developed by the European Commission to provide a standardized framework for assessing the environmental impacts of products and organizations. It comprises two key components:

1) Product Environmental Footprint (PEF): Measures the environmental impacts of products (goods or services) throughout their entire life cycle.
2) Organization Environmental Footprint (OEF) – not relevant for the HemiCoat project: Evaluates the overall environmental impact of an organization, taking into account all its activities and outputs.

The EF method aligns with the ISO 14040 and ISO 14044 standards, ensuring a comprehensive life cycle evaluation while being designed to enhance consistency, reproducibility, and comparability in environmental assessments across industries.[14] Noteworthy, the HemiCoat LCA boundaries define a Cardle-to-Gate approach and, therefore, do not consider end-of-life scenarios or end-of-life allocation approaches and formulas.[15]

3.5.3. Impact categories

The EF method typically focuses on calculating environmental impacts at the midpoint level, not the endpoint. All 16 impact categories/recommended methods covered by the EF (JRC technical reports, 2018)[16] are considered to evaluate the environmental impact of the HemiCoat process flow.

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[14] European Commission, “Life Cycle Assessment & the EF Methods.”

[15] Allacker et al., “The Search for an Appropriate End-of-Life Formula for the Purpose of the European Commission Environmental Footprint Initiative.”

[16] Fazio et al., “Supporting Information to the Characterisation Factors of Recommended EF Life Cycle Impact Assessment Methods.”

Table 2 lists and describes the impact categories at the midterm level.

Table 2. Environmental impact categories as suggested in the JRC Technical Reports: Supporting information to the characterization factors of recommended EF LCIA methods.[17]

Impact category	Indicator	Unit
Climate change	Radiative forcing as Global Warming Potential (GWP100)	kg CO_2 eq
Ozone depletion	Ozone Depletion Potential (ODP)	kg CFC-11 eq
Human toxicity, cancer effects	Comparative Toxic Unit for humans (CTU_h)	CTU_h
Human toxicity, non-cancer effects	Comparative Toxic Unit for humans (CTU_h)	CTU_h
Particulate matter/Respiratory inorganics	Human health effects associated with exposure to $PM_{2.5}$	Disease incidences
Ionizing radiation, human health	Human exposure efficiency relative to U^{235}	kBq U^{235}
Photochemical ozone formation	Tropospheric ozone concentration increase	kg NMVOC eq
Acidification	Accumulated Exceedance (AE)	mol H^+ eq
Eutrophication, terrestrial	Accumulated Exceedance (AE)	mol N eq
Eutrophication, aquatic freshwater	Fraction of nutrients reaching freshwater end compartment (P)	kg P eq
Eutrophication, aquatic marine	Fraction of nutrients reaching marine end compartment (N)	kg N eq
Ecotoxicity freshwater	Comparative Toxic Unit for ecosystems (CTU_e)	CTU_e
Land use	Soil quality index (Biotic production, Erosion resistance, Mechanical filtration	Dimensionless, aggregated index of: kg biotic production/ (m^{2*}a) kg soil/ (m^{2*}a)
Water use	User deprivation potential (deprivation-weighted water consumption)	kg world eq. deprived
Resource use, minerals and metals	Abiotic resource depletion (ADP ultimate reserves)	kg Sb eq
Resource use, energy carriers	Abiotic resource depletion – fossil fuels (ADP-fossil)	MJ

Focusing the HemiCoat LCIA on these midpoint indicators offers several advantages, primarily due to their simplicity and the availability of well-established calculation methodologies. Midpoint indicators, such as global warming potential, acidification, and eutrophication, are relatively simple to quantify with a lower level of uncertainty than endpoint indicators. Yet, midterm indicators provide a detailed analysis of specific environmental impacts of a product's life cycle. With the selected indicators, a clearer understanding of how different processes contribute to specific environmental concerns is described, making them valuable for identifying hotspots and targets for improvement. The selected indicators are widely recognized and standardized, therefore allowing for comparability across studies and sectors. Overall, by focusing on midpoints, LCA practitioners can obtain actionable insights without the complexity and uncertainty associated with endpoint assessments, which involve broader, more speculative long-term consequences. The selected impact categories are thus particularly valuable for product development, policy formulation, and environmental management decision-making.

[17] Fazio et al.

However, since LCA models inherently rely on a variety of assumptions, it becomes essential to employ methods for assessing uncertainty in both LCI and impact assessment. These methods are crucial for effectively conveying the influence of such assumptions on the results, ensuring more accurate and transparent decision-making.

3.5.4. Uncertainty analysis and data quality

Uncertainty analysis is a crucial aspect of LCA studies, significantly enhancing the reliability and credibility of the results. By systematically identifying, characterizing, propagating, and understanding uncertainties, practitioners can better assess the environmental impacts of products and processes. Uncertainty can arise from various sources, including quantity, model structure, and context, each requiring specific methods for effective management. Techniques such as probability distributions, Monte Carlo sampling, and sensitivity analysis help quantify and propagate uncertainties, providing a clearer picture of potential variations in LCA outcomes. Effective communication of these uncertainties, through qualitative and quantitative assessments, ensures that stakeholders are well-informed about the confidence and limitations of the results. Recommendations for different levels of uncertainty treatment, tailored to the practitioner's expertise, further support robust decision-making.[18]

In the openLCA software, all data quality systems adhere to a pedigree matrix framework, where data quality indicators are assessed and classified from good to poor, in 5 grades, and for the following 5 categories:

- Reliability
- Completeness
- Temporal correlation
- Geographical correlation
- Further technological correlation

Based on the pedigree matrix, the openLCA tool facilitates the implementation of a Monte Carlo Simulation (MCS) by utilizing per-exchange uncertainty data (data quality) to evaluate uncertainty. The MCS output provides key statistical metrics, including the mean result, standard deviation, 5^{th} and 95^{th} percentile boundaries, and the median value of the simulated results. In principle, MCS randomly alters input data using predefined uncertainty distributions. This approach accounts for input data variability, generating a range of possible outcomes, each associated with a specific uncertainty distribution. Typically, thousands of iterations are performed to ensure the robustness and reliability of the results.[19]

3.6. Life cycle comparison in HemiCoat

Comparing the HemiCoat attributional LCA with LCAs from the literature is essential for validating results, contextualizing findings, and benchmarking environmental performance. Such comparisons enable the identification of methodological differences, variations in system boundaries, and key assumptions that may influence outcomes. Furthermore, they facilitate the recognition of industry best practices, emerging trends, and areas for potential improvement, thereby enhancing the robustness of the analysis and supporting more informed decision-making in sustainability research and practice.

[18] Igos et al., "How to Treat Uncertainties in Life Cycle Assessment Studies?"
[19] Greendelta GmbH, "Monte Carlo Simulation - openLCA 2 Manual."

When conducting a comparative LCA in accordance with ISO 14044, the study's scope must be defined to ensure the equivalence of the systems under comparison. This is achieved by establishing methodological parameters, including performance criteria, system boundaries, data quality requirements, allocation procedures, and decision rules for evaluating inputs, outputs, and impact assessment.[20] For the HemiCoat project, within the framework of a Cradle-to-Gate perspective, two types of sustainability comparisons are planned, based on:

1) Technically identical product(s).
2) Functionally equivalent product(s).

3.6.1. LCA comparison based on technically identical product(s)

For the comparison based on *1) Technically identical product(s)*, LCA module 1 of the HemiCoat project is assessed against a reference LCA from literature, in which IA is produced from pretreated wheat straw in a biorefinery approach.[21] Herein, the product, defining the FU = 1 kg of IA with a purity of 99 %, is identical. **Figure 8** displays the simplified LCIs of (**a**) the HemiCoat LCA module 1 and (**b**) the reference LCA, indicating the difference between them.

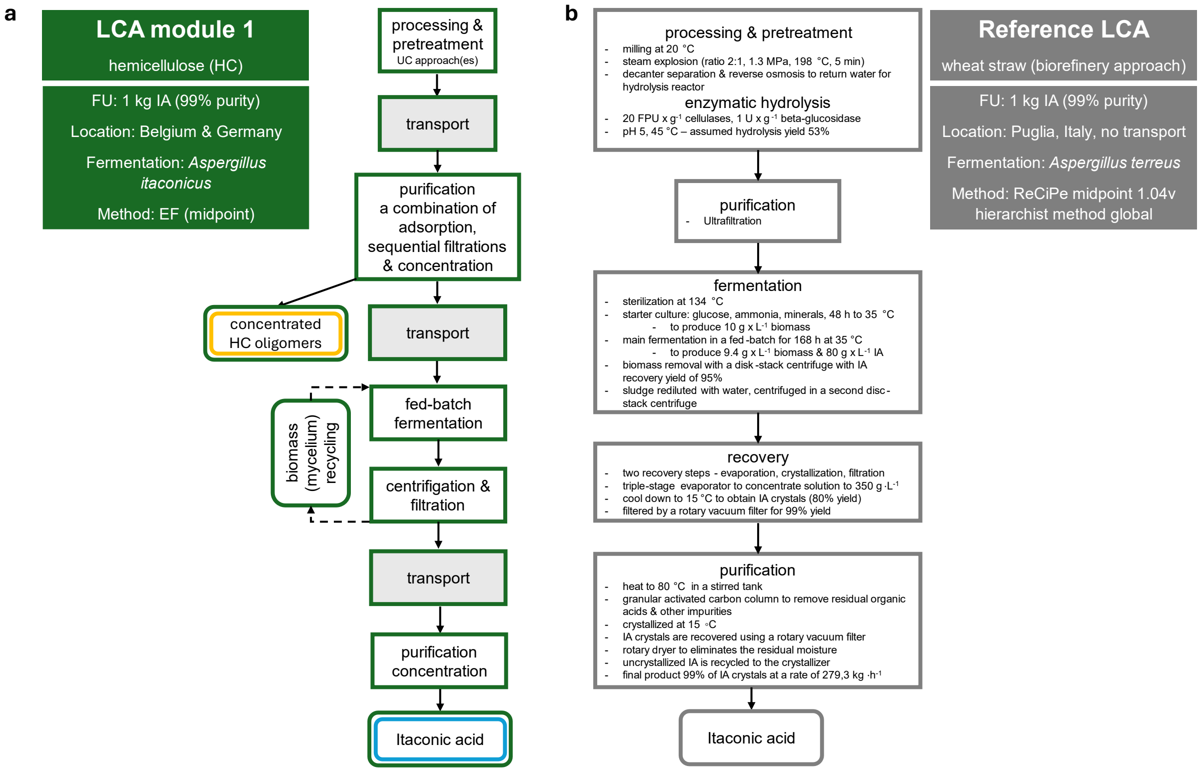

Figure 8. Life cycle comparison for the production of Itaconic acid.

Process flows implemented in the LCIs for the production of 1 kg of IA with a purity of 99 % based on **(a)** the HemiCoat LCA module 1 and **(b)** a reference LCA.[22]

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[20] Cottafava et al., "Requirements for Comparative Life Cycle Assessment Studies for Single-Use and Reusable Packaging and Products."

[21] Rebolledo-Leiva, Moreira, and González-García, "Environmental Assessment of the Production of Itaconic Acid from Wheat Straw under a Biorefinery Approach."

[22] Rebolledo-Leiva, Moreira, and González-García.

Another comparison based on *1) Technically identical product* is the production of polyitaconic acid (PIA). Nuss & Gardner describe corn-derived PIA of 1 kg of polymer and compare the results with the production of fossil-based polyacrylic acid (PAA).[23] This work can be directly compared to the results gained in the HemiCoat LCA following the process flows for the production of PIA, as shown in **Figure 9**.

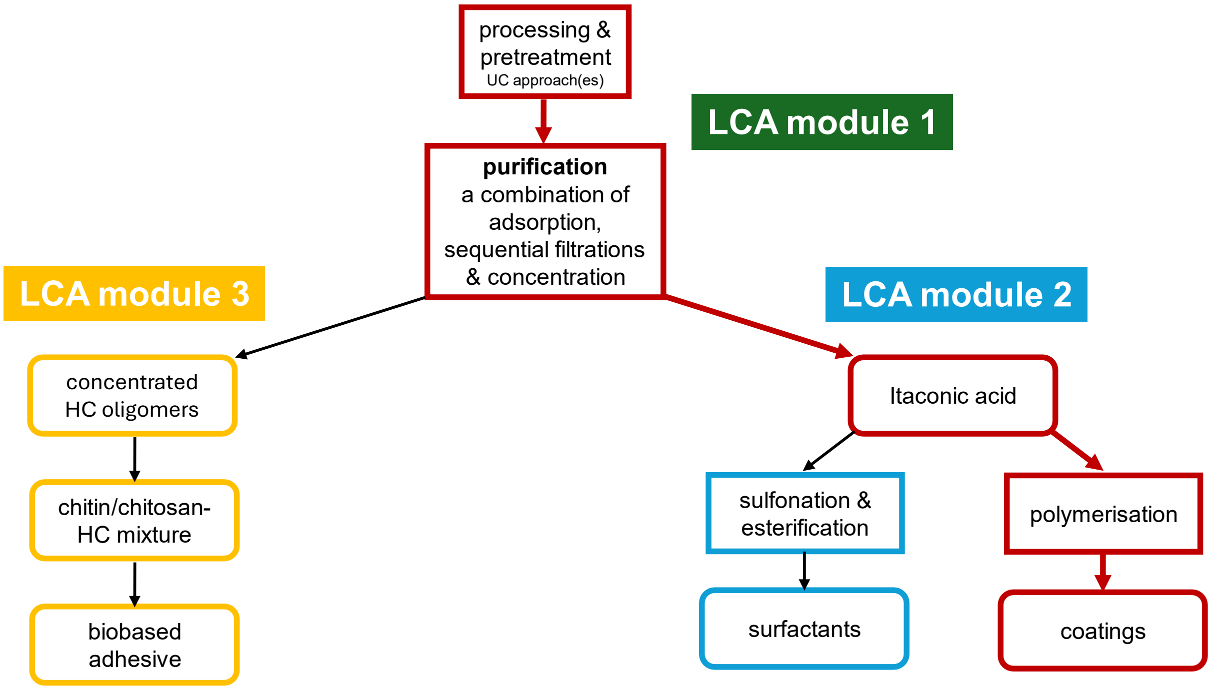

Figure 9. Process flowchart in HemiCoat for the production of polyitaconic acid (PIA).

The process branch for the production of PIA in the HemiCoat project is framed in red, leading to biobased coatings after IA polymerization. Herein, parts of LCA modules 1 & 2 are included.

Comparing the biorefinery approach to produce IA from wheat straw[24] or the PIA production from softwood[25] as described in literature with the process developed in the HemiCoat project ensures that variations in environmental impact, efficiency, and sustainability are exclusively attributable to differences in production processes rather than discrepancies in product functionality. Therefore, *1) Technically identical product* comparison minimizes methodological bias and enhances the robustness of the analysis and, thus, allows a more precise evaluation of technological advancements and sustainability improvements, supporting data-driven decision-making in process optimization and resource efficiency.

3.6.2. LCA comparison based on functionally equivalent product(s)

For the remaining aspects of the project, no reference systems offering a technically identical product are available in the existing literature. As a result, comparisons with established systems must focus on *2) Functionally equivalent product(s)*. This applies, e.g. to a study by Morão & de

[23] Nuss and Gardner, "Attributional Life Cycle Assessment (ALCA) of Polyitaconic Acid Production from Northeast US Softwood Biomass."

[24] Rebolledo-Leiva, Moreira, and González-García, "Environmental Assessment of the Production of Itaconic Acid from Wheat Straw under a Biorefinery Approach."

[25] Nuss and Gardner, "Attributional Life Cycle Assessment (ALCA) of Polyitaconic Acid Production from Northeast US Softwood Biomass."

Bie, in which polylactic acid (functionally equivalent to PIA) is produced from sugarcane.[26] In the field of biobased surfactants, several reference systems are available[27] allowing the LCA comparison based on *2) Functionally equivalent product(s)*. The same applies to biobased adhesives. **Table 3** shows selected studies for both classes.

Table 3. Reference literature on LCA studies of functionally equivalent biobased adhesives or surfactants.

Title and reference	Target product	Comparative criteria
A compilation of life cycle studies for six household detergent product categories in Europe: the basis for product-specific A.I.S.E. Charter Advanced Sustainability Profiles[28]	Manual dishwashing detergents, powder and tablet laundry detergents, window glass trigger spray cleaners, bathroom trigger spray cleaners, acid toilet cleaners, and bleach toilet cleaners	Cradle-to-Grave, ReCiPe end point using hierarchist perspective with European normalization data (Year 2000)
New and updated life cycle inventories for surfactants used in European detergents: summary of the ERASM surfactant life cycle and ecofootprinting project[29]	15 surfactants (anionic, non-ionic, cationic, amphoteric) and 17 precursors	Cradle-to-Gate, energy sources and demand, GWP100
The Role of Environmental Evaluation within Circular Economy: An Application of Life Cycle Assessment (LCA) Method in the Detergents Sector[30]	Ecological detergent “Ri-Detersivo” (Tea Natura), mainly composed of regenerated vegetable oils	Cradle-to-Gate
Cradle-to-gate Life Cycle Assessment of bio-adhesives for the wood panel industry. A comparison with petrochemical alternatives[31]	Four different bio-adhesives as alternatives, derived from biopolymers, e.g. protein (soy), lignin (Kraft & Organosolv), and tannin	Cradle-to-Gate, ReCiPe midpoint
Comparative life cycle assessment for the manufacture of bio-detergents[32]	Bio-multipurpose liquid detergent (bio-detergent containing anionic plant-based surfactants)	midpoint, optional endpoint impact categories
Eco-efficiency assessment of liquid dishwashing detergents[33]	Three detergents produced in Teresina-Piauí-Brazil	Cradle-to-Gate, ReCiPe midpoint

[26] Morão and De Bie, “Life Cycle Impact Assessment of Polylactic Acid (PLA) Produced from Sugarcane in Thailand.”
[27] ERASM research platform, “ERASM - Publications.”
[28] Golsteijn et al., “A Compilation of Life Cycle Studies for Six Household Detergent Product Categories in Europe.”
[29] Schowanek et al., “New and Updated Life Cycle Inventories for Surfactants Used in European Detergents.”
[30] Lucchetti et al., “The Role of Environmental Evaluation within Circular Economy.”
[31] Arias et al., “Cradle-to-Gate Life Cycle Assessment of Bio-Adhesives for the Wood Panel Industry. A Comparison with Petrochemical Alternatives.”
[32] Villota-Paz, Osorio-Tejada, and Morales-Pinzón, “Comparative Life Cycle Assessment for the Manufacture of Bio-Detergents.”
[33] De Moura and Da Silva, “Eco-Efficiency Assessment of Liquid Dishwashing Detergents.”

Additionally, sodium dodecyl sulfate (SDS, CAS 151-21-3, also sodium lauryl sulfate) is selected as a reference. SDS is the archetypal anionic, single-chain surfactant whose critical micelle concentration, adsorption kinetics, and denaturing power have been measured for decades. Moreover, its environmental profile (energy use, GHG emissions, eutrophication, ecotoxicity, end-of-life biodegradation[34]) is available and well documented.[35,36,37] Using SDS as the reference for the LCA in HemiCoat provides a well-characterized[38] baseline with numerous industrial applications, ensuring data quality and replicability for the environmental evaluation. Representing a highly pure, easily available, and low-cost surfactant with high cleaning power, but strong protein denaturation, with well-established analytical properties, SDS directly addresses regulators' and formulators' green-chemistry criteria. Finally, established conversion factors and data relationships for SDS, such as the link between surface tension and critical micelle concentration (CMC), allow for validating experimental results before applying them to broader environmental assessments. This helps reduce errors and uncertainty in the analysis, ensuring that any observed benefits of the bio-based surfactant reflect real-life cycle improvements rather than inconsistencies in methodology, and hence minimizes methodological noise, maintaining a clear emphasis on real-life performance of the bio-based surfactants from the HemiCoat process flow.

Comparing the HemiCoat LCA with studies based on *2) Functionally equivalent product(s)* ensures that the environmental performance of the studied processes can still be evaluated within a relevant context. The availability of reference systems for biobased surfactants and adhesives provides a foundation for benchmarking HemiCoat's ecological performance through the results gained in LCA modules 2 and 3 and enables a more comprehensive assessment of the sustainability and efficiency of the investigated production processes in the project.

[34] Zicarelli et al., "Effects of a Common Surfactant Sodium Lauryl Sulfate on Early Life Stages of Two Fish and One Amphibian Species."

[35] Khan, Bawankar, and Gahalod, "Life Cycle Assessment of SLS And SLES (Sodium Lauryl Sulfate And Sodium Laureth Sulfate) Product."

[36] Villota-Paz, Osorio-Tejada, and Morales-Pinzón, "Comparative Life Cycle Assessment for the Manufacture of Bio-Detergents."

[37] Asio et al., "Sodium Lauryl Sulfate and Its Potential Impacts on Organisms and the Environment: A Thematic Analysis."

[38] "Safety Data Sheet Sodium Dodecyl Sulfate."

4. Conclusion, strategic recommendations & outlook

The deliverable *D1.4 Interim report on definitions, settings, and system for LCA* describes definitions and settings for the attributional LCA in HemiCoat, thus representing the preparatory work for *D1.5 LCA of hemicellulose oligomers and itaconic acid-based products*. In the next months, data collection will be completed, and a first set-up of the LCA model is envisaged. An updated version, including the final definitions and settings for the HemiCoat LCA will be provided in *D1.5* in M24 (August 2026). The findings of the HemiCoat LCA will highlight the critical role of cross-border industrial collaboration in advancing bio-based coating and surfactant solutions as well as adhesives. Several key insights are expected to emerge from the analysis that will enable stakeholders to make decisions on the extent to which hemicellulose-containing hydrolysate from by-products used following the HemiCoat process flow and contribute to a sustainable supply of the targeted coating, surfactant, and adhesive materials. Overall, we hope that this approach will contribute to improved resource efficiency and long-term sustainability in industrial applications.

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