



CALiMERO

IMPROVING BIO-BASED INDUSTRIES LIFE CYCLE SUSTAINABILITY

D3.5

Definition of relevant socio-economic indicators to include in LCSA of target bio- based industries

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LIST OF ACRONYMS

API	Application Program Interface	LCSA	Life Cycle Sustainability Assessment
BIC	Bayesian Information Criterion	LCT	Life Cycle Thinking
CAPEX	Capital Expenditures	MF	Mass Flow
CAS	Chemical Abstracts Service	MFCA	Material Flow Cost Accounting
CF	Characterization Factor	ML	Machine Learning
cLCC	conventional Life Cycle Costing	MOO	Multi-Objective Optimization
CLP	Classification, Labelling and Packaging	MSE	Mean Squared Error
DNEL	Derived No Effect Level	NGO	Non-Governmental Organization
ECF	Exposure Concentration Factor	NPV	Net Present Value
ECHA	European Chemicals Agency's	OECD	Organization for Economic Co-operation and Development
EF	Environmental Footprint	OEL	Occupational Exposure Limit
eLCC	environmental Life Cycle Costing	OHS	Occupational Health and Safety
ETS	Emission Trading System	OPEX	Operational Expenditures
EoL	End-of-life	PEF	Product Environmental Footprint
EU	European Union	PHF	Person-Hours Factor
feLCC	full environmental Life Cycle Costing	PP	Payback Period
FTE	Full Time Equivalent	PPE	Personal Protective Equipment
FU	Functional Unit	PSIA	Product Social Impact Assessment Handbook
GMM	Gaussian Mixture Model	PSILCA	Product Social Impact Life Cycle Assessment
HF	Hazard Factor	REACH	Registration, Evaluation, Authorization and Restriction of Chemicals Regulations
ILOSTAT	International Labor Statistics	RS	Reference Scale
IOTs	Input-Output Tables	SDG	Sustainable Development Goal
IP	Impact Pathway	SHDB	Social Hotspot Database
IRR	Internal Rate of Return	S-LCA	Social Life Cycle Assessment
JCP	Job Creation Potential	sLCC	social Life Cycle Costing
JRC	Joint Research Centre	SSbD	Safe and Sustainable by Design
LCA	Life Cycle Assessment	TCO	Total Cost of Ownership

LCC	Life Cycle Costing	TEA	Techno-Economic Assessment
LCI	Life Cycle Inventory	UN	United Nations
LCIA	Life Cycle Impact Assessment	USD	United States Dollars
LCOP	Levelized Cost of Production	WH	Working Hours

PROJECT INFORMATION

Project full title: Industry Case Studies Analysis to Improve Environmental Performance and Sustainability of Bio-based Industrial Processes

Acronym: CALIMERO

Call: HORIZON-CL6-2021-ZEROPOLLUTION-01

Topic: HORIZON-CL6-2021-ZEROPOLLUTION-01-06 - Increasing the environmental performance of industrial processes in bio-based sectors: construction, woodworking, textiles, pulp and paper and bio-chemicals

Start date: 1st July 2022

Duration: 48 months

List of participants:

Partner No.	PARTICIPANT ORGANIZATION ACRONYM
1 (Coord.)	Contactica CTA
2	WeLOOP WELOOP
3	European Cellulose Insulation Association ECIA
4	Swedish Environmental Research Institute IVL
5	Neovili NEOVILI
6	Cesefor CESEFOR
7	Luxembourg Institute of Science and Technology LIST
8	Technical University of Denmark DTU
9	Techtera TECHTERA
10	Essity ESSITY
11	BIM Kemi AB BIMKEMI
12	Ereks garment EREKS

DELIVERABLE DETAILS

Document Number:	D3.5
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Dissemination level:	PU – Public
Period:	PR2
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Task:	T3.4 – Definition of methodology to assess socio-economic impacts

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Abstract:	<p>In the context of the CALIMERO project, this deliverable aims at proposing social and economic indicators to be integrated in the form of a Life Cycle Sustainability Assessment (LCSA) to be applied into 5 different bio-based sectors (textiles, construction, woodworking, bio-chemicals and pulp and paper). For this purpose, following the internal agreement of the consortium, a set of socio-economic aspects and indicators have been selected to be considered together with the Product Environmental Footprint (PEF) methodology and to be integrated in a Multi-Objective Optimization (MOO) framework to be further developed.</p> <p>Among the Social LCA (S-LCA) indicators and aspects selected are the Job Creation Potential (JCP), Occupational Exposure Limits (OELs) linked with Occupational Health and Safety (OHS), as well as the proposal of novel human toxicity Characterization Factors (CFs). Regarding the latter, CFs from 49 chemicals used in the CALIMERO case studies were developed for USEtox using Machine Learning (ML). Two ML models were apprehended (XGBoost and Gaussian process), of which mainly XGBoost showed the more adequate predictive capability. In the case of ProScale, a combination of new data collection and ML for the H-phrases, based on already-existing models, was apprehended to obtain novel CFs. Starting from 991 chemicals, eventually 62 CFs were derived.</p> <p>Concerning the economic domain, the Net Present Value (NPV) or the Internal Rate of Return (IRR) were chosen to be evaluated, among others economic indicators. The methodologies for their calculation have been described in detail, as well as the provision of calculation tools as annexes with the purpose of facilitating its reproducibility beyond the project scope. However, it was also decided to go one step further in order to add novelty to the report by methodologically refining some indicators or proposing new ones to be implemented in future iterations.</p> <p>The methodologies presented here have proved to be useful in fulfilling the mission of the CALIMERO project, but once again the lack of consensus on the socio-economic life cycle approach is confirmed in order to obtain more standardized and easily applicable methodologies, although this document represents a good starting point for the integration of the life cycle approach with the MOO framework in a bioeconomy context.</p>

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1 INTRODUCTION

1.1 Context

The concept of "sustainable development" was officially introduced in 1987 by the Brundtland Report, which defined it as a development that "meets the needs of the present without compromising the ability of future generations to meet their own needs" (Hasegawa et al., 2022). The report emphasized the need for economic growth that is aligned with the protection of the environment and social welfare. Building upon Brundtland Report, the "Agenda 21" was established in 1992 during the Earth summit in Rio de Janeiro (Brazil) to operationalize the theoretical concept of sustainable development (Lafferty and Eckerberg, 2013). In 2015, a new framework was developed by the United Nations (UN) General Assembly called Agenda 2030, which has been adopted by all UN member states and it encompasses a set of 17 Sustainable Development Goals (SDGs) and associated indicators across the three dimensions of sustainability: (i) environment, (ii) society and (iii) economy, aiming to facilitate the implementation of daily actions towards sustainability (United Nations, 2015).

In this context, it is possible to categorize some sectors as "more sustainable" than others, depending on several factors such as the raw materials required, the type and intensity of production practices, or even contextual variables. In the case of bioeconomy, this includes various activities that use biological resources to produce goods and services. It is important to note, however, that the bioeconomy sector is not inherently sustainable. This is because, although it offers the potential for more environmentally friendly practices, the specific design, careful monitoring and thorough evaluation of bioeconomy activities are crucial to the implementation of a sustainable bioeconomy (Aguilar et al., 2019).

There are several analytical tools to properly assess sustainability, among which Life Cycle Sustainability Assessment (LCSA) stands out for its holistic perspective (considering the life cycle of a product or service) (Valdivia and Sonnemann, 2024). In addition, LCSA is designed to evaluate the three pillars of sustainability, which can be achieved by integrating the methodologies of Life Cycle Assessment (LCA), Life Cycle Costing (LCC), and Social Life Cycle Assessment (S-LCA). In practice, this commonly boils down to executing all latter three separately, with similar goal and scope, and then aggregate the results (Valdivia et al., 2021). Yet, alternatives have been conceived and to a limited extent applied (Schaubroeck and Rugani, 2017). Nevertheless, because of its life cycle approach and the interrelated assessment of the three pillars, LCSA holds great promise for assessing the sustainability of activities and identifying potential trade-offs between economic, environmental and social dimensions. Although LCA is a well-established methodology with international standards outlining its principles and framework (i.e., ISO 14040), along with specific requirements and guidelines (i.e., ISO 14044) (ISO, 2006a, 2006b), LCC and S-LCA are still in the process of maturing to establish a consensual methodological framework.

In this situation, due to the limited methodological context of LCC and S-LCA, most LCSAs conducted to date have focused solely on the environmental dimension of sustainability (Larsen et al., 2022), leaving economic growth and social well-being unattended. Therefore, the development of clear and agreed methodologies for LCC and S-LCA is essential to strengthen the practical application of LCSA as a whole and to facilitate alignment with the broader SDGs set by the international community. In this way, all sectors of the bioeconomy can benefit to ensure a smooth and sustainable transition to the bioeconomy paradigm.

1.2 Aim and objectives

The CALIMERO project, funded by Horizon Europe, aims to enhance sustainability in industrial bio-based sectors by improving existing sustainability assessment methodologies. This report addresses the social and economic dimensions of sustainability to a certain degree to foster a holistic evaluation of industrial activities. Its main purpose is to outline a methodology for integrating certain socio-economic impacts into the assessment of bio-based industries using a Life Cycle Thinking (LCT) approach. Specifically, a limited set of

social and economic indicators was proposed to evaluate the 5-target industrial bio-based sectors within the CALIMERO project, which include: (i) construction, (ii) textiles, (iii) woodworking, (iv) bio-chemicals, and (v) pulp and paper. The list of socio-economic indicators/aspects addressed is presented in **Table 1**. Likewise, this is accompanied by a detailed description of their rationale and data requirements, as well as methodological recommendations for their effective implementation in the following sections.

The reasoning behind the focus on or choice of one or another indicator or socio-economic aspect was made through agreements in the project consortium, which is supported by two main reasons. On the one hand, the previous expertise of the academic partners (i.e., life cycle practitioners) to ensure the correct applicability of the socio-economic analysis. On the other hand, the usefulness of those in the context of the CALIMERO project, which must be compatible with the Multi-Objective Optimization (MOO) approach developed in WP4 to be used later in WP5. In this sense, once a series of solutions to improve sustainability has been identified (T5.1 and T5.2), their potentials will be further demonstrated in CALIMERO task T5.3, and its forthcoming deliverable (D5.3), following a holistic perspective of sustainability, integrating within the MOO framework not only environmental aspects by using LCA indicators, but also additional LCC and S-LCA ones.

Notwithstanding, apart from complying with the aim of the CALIMERO project, several novel aspects have been also addressed with the goal of providing added-value features to this deliverable. In this regard, some examples are in relation to the agreement of refining already implemented methodologies of the S-LCA (see **Section 2.3.1**), as well as the proposal of new indicators for broadening the current scope of the LCC (see **Section 3.2.5**). Lastly, in order to facilitate the applicability of the life cycle socio-economic methodologies presented, two calculator tools have been developed in the form of Excel files.

Table 1. Set of socio-economic indicators/aspects considered in the CALIMERO project.

Sustainability dimension	Indicator/aspect
Society	Job Creation Potential (JCP)
	Occupational Exposure Limits (OELs) indicator
	Toxicity Characterization Factors (CFs) from USEtox and ProScale
Economy	Life Cycle Cost (LCC)
	Net Present Value (NPV)
	Levelized Cost of Production (LCOP)
	Internal Rate of Return (IRR)
	Payback period (PP)
	Environmental externalities
	Economic aspects beyond profitability (not covered within the CALIMERO case studies): <ul style="list-style-type: none"> • <i>Stability</i> • <i>Autonomy</i> • <i>Productivity</i> • <i>Customers</i> • <i>Innovation</i>

1.3 Report structure

This report uses a systematic approach to achieve its overarching goal of establishing a life cycle methodology for assessing socio-economic impacts that can be easily integrated into a MOO framework. It begins by presenting key findings from a concise state-of-the-art review of social impact assessment methods within the specified bio-based industries (**Section 2**). This initial section covers the selection of certain relevant social indicators on which to focus, ensuring their applicability within the project's context, and outlines the necessary steps and data requirements for their development. The subsequent section mirrors the first but focuses on economic indicators (**Section 3**), starting with an exploration of the current landscape of economic evaluation methodologies, followed by a detailed description of the proposed economic indicators. Lastly, the conclusions and future prospects of the report are brought forward in **Section 4**. two calculator tools facilitate the work in relation to the JCP estimation (*Annex A. Job Creation Potential calculator tool*) and the evaluation of the LCC indicators chosen (*Annex B. Life Cycle Costing indicators calculator tool*).

2 SOCIAL EVALUATION OF TARGET BIO-BASED INDUSTRIES

2.1 State-of-the-art

S- S-LCA is a methodology to assess the social impacts of products and services throughout their life cycle, from the extraction of raw materials to the End-of-Life (EoL) phase (UNEP et al., 2020). The UNEP/SETAC Life Cycle Initiative's guidelines on S-LCA, published in 2009 and updated in 2020 and 2021, are the primary references in the field, setting out the basic concepts of social impact assessment from a life cycle perspective and providing technical guidance to practitioners on how to conduct an S-LCA in a practice-oriented way, e.g., through the provision of methodological sheets (UNEP et al., 2021). This work has inspired other relevant publications, such as the *Product Social Impact Assessment Handbook* (PSIA), which narrows down the broad scope of UNEP/SETAC Life Cycle Initiative guidelines to a more specific operational set of indicators (Goedkoop et al., 2020), and the *Social Life Cycle Metrics for Chemical Products*, which tailors the methodology to the chemical sector (World Business Council for Sustainable Development, 2016). A more detailed historical trajectory of S-LCA methodology can be found in D1.3 (*Characterization of the main methodological gaps in sustainability assessment of bio-based sectors*) of the CALIMERO project. Additionally, the latter report (D1.3) provides an overview of the main methodological gaps encountered when applying S-LCA to bio-based industries. These gaps formed the basis for the definition of the methodological approach that will be adopted within the CALIMERO project to assess the social impacts of selected case studies, as explained in detail below.

2.2 Methodological approach of social life cycle assessment

SLCA combines the modeling and systematic assessment approach of LCA on social science to evaluate social impacts in line with ISO 14040 and ISO 14044 standards. Due to its focus on people, social concerns are conventionally arranged among 6 stakeholder categories: children, workers, local community, society, consumers, and value chain actors. Resembling LCA, S-LCA is performed following 4 main steps, including goal and scope definition, inventory analysis, impact assessment and interpretation.

Step 1. Goal and scope definition

Firstly, a clear purpose of the assessment should be defined, along with its scope and associated methodological implications, mainly the Functional Unit (FU), reference flow, target stakeholders and system boundaries. These methodological assumptions, especially the FU and the reference flow, should be the same or equivalent among the three life cycle methods to allow the integration of the three aspects of sustainability in a unified assessment (i.e., the LCSA).

Step 2. Inventory analysis

At this stage, an inventory is compiled of all the product flows, waste flows and social inventory indicators (flows, pressures or conditions) of the defined product life cycle, normalized to the FU. Concerning quantification and defining product flow and waste flows among processes, the same approach can be taken for any life cycle method (Schaubroeck and Benetto, 2024). Besides social inventory indicators, there are some unique features to the LCI of S-LCA. An activity variable is commonly defined to aid in the assessment. Activity variables are measures that reflect the distribution of “activity” for the system under study along its unit processes, giving an idea of the relative importance of each unit process in the overall system and relate impacts to it, e.g. worker-hours can be seen as representing a scaling factor for social issues, especially those for workers as stakeholder category. Social inventory indicators are simple variables (e.g., salary or number of accidents) that may indicate the status of a particular issue, life cycle stage, or process, but they are not always scalable. **Figure 1** depicts an example of Life Cycle Inventory (LCI) illustrating the function of activity variables and social inventory indicators. Primary data from life cycle actors as well as background databases, e.g., Input-Output Tables (IOTs), apart from S-LCA dedicated databases such as SHDB (Social Hotspot Database), can be used. IOTs consist of tables that reflect the (economic) transactions between sectors or product groups within an economy (Suh and Huppel, 2005).

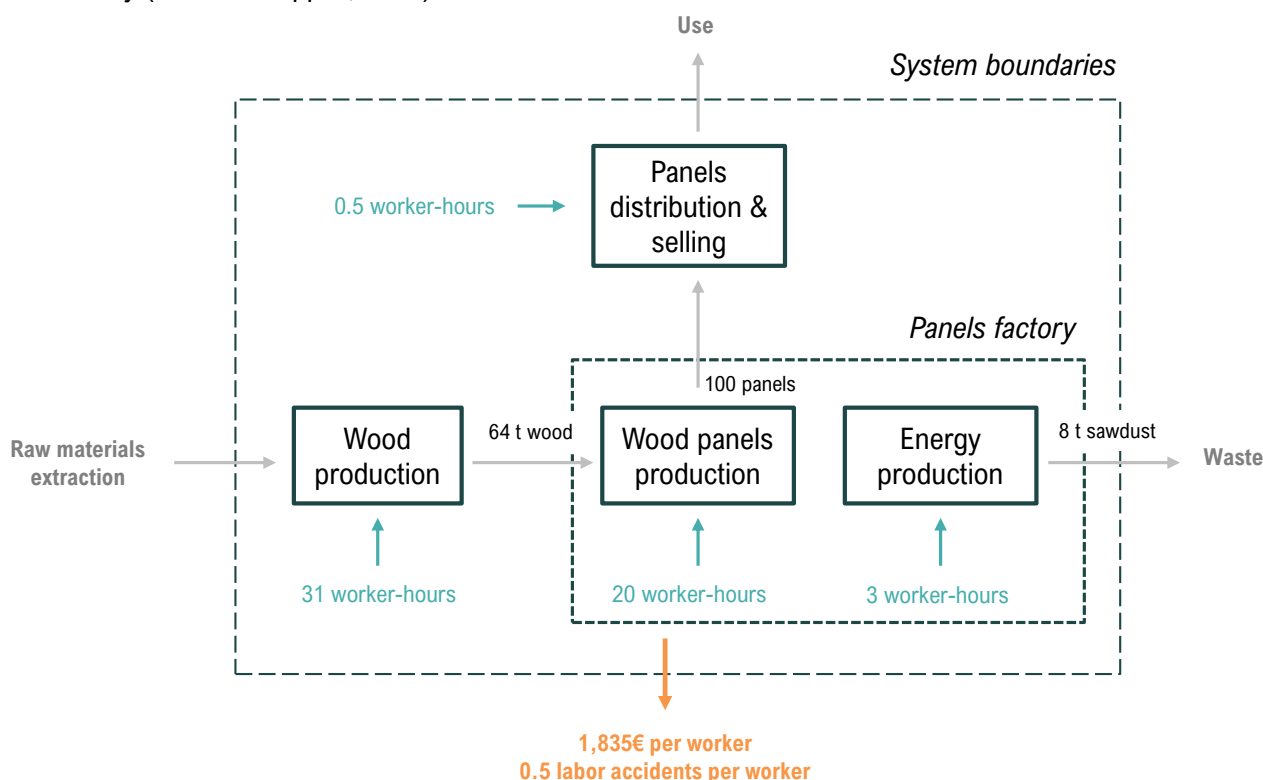


Figure 1. Illustration of the difference between the activity variable (in blue) and the social inventory indicator (in orange) using a fictitious example of panel production in the woodworking sector. Figure adapted from UNEP (2020).

Step 3. Impact assessment

Two impact assessment approaches can be followed in S-LCA: (i) the Reference Scale (RS) approach or (ii) the Impact Pathway (IP) approach. While the former approach assesses the social performance using specific reference points based on experts' judgement and available information, the latter is based on a causal relationship between the product system and the social impacts, which is more in line with LCA methodology and thus, enables better complementation with the environmental assessment for a holistic sustainability assessment (Alvarenga et al., 2021). For this reason, the IP approach has been adopted within the CALIMERO project. The impact categories, i.e., the categories of social impact or concern, in association with the method

for their characterization should be defined in this analysis step.

Once all the data is collected, the next step consists in quantifying the magnitude and significance of the potential social impacts of a product system throughout its life cycle. For this, **Section 2.3** presents the social indicators that will be analyzed within the CALIMERO project.

Step 4. Interpretation

Finally, the results should be reviewed and discussed to derive conclusions, recommendations and final decisions in accordance with the originally defined objective and scope. At this stage, the limitations of the study, such as the type and quality of the data used, or any assumptions that may lead to underestimations of the final results, should also be pointed out.

2.3 Selected social indicators

Based on an analysis of a variety of sources, including related projects, such as ORIENTING, in relation to its deliverable D1.2 (Alvarenga et al., 2021), specialized databases (e.g., the SHDB), or the Product Social Impact Life Cycle Assessment (PSILCA)), and a recent body of peer-reviewed articles and policies; a set of six main gaps of S-LCA methodology were identified and categorized by typology: modelling or conceptual (see **Table 2** obtained from D1.3).

Table 2. Main methodological gaps of the Social Life Cycle Assessment identified (collected from D1.3 Characterization of the main methodological gaps in sustainability assessment of bio-based sectors - CALIMERO project).

#	Type of gap	Gap	Possible solution(s)
1	Modelling	Some of the specificities of bio-based systems are not addressed by the current S-LCA methodologies	Propose new social impact categories or modify existing ones to adapt them to the specificities of bio-based systems
2		Most S-LCA studies are focused on the production side (worker stakeholder) and the energy sector (e.g., bioenergy)	Release the data and methodological constraints to carry out more comprehensive social assessments
3	Conceptual	Lack of inclusion of key concepts related to (bio-)economy strategies (e.g., job creation or skills training)	To establish a consensus between (bio)economy strategies and S-LCA methodologies
4		Several LCT issues, such as FU definition, modeling of background processes or sensitivity analysis of the results	Standardized life cycle perspective
5		No relation between social labels and S-LCA studies	Creation of new integrative certifications and policies

One highlighted issue is the lack of specificity in defining stakeholders, leaving some relevant social groups of the bio-based systems, such as smallholders, not well represented. In addition, the omission of important social aspects such as employment opportunities and training programs are a cause for concern. Moreover, the limited availability of quantitative social indicators makes it difficult to integrate the social dimension with the environmental and economic spheres, which hinders a more holistic analysis of the sustainability performance. In response to these methodological limitations, the following indicators/aspects are proposed as focus for the selective assessment of the social impact of the bio-based industries to be analyzed within the CALIMERO project:

- i) Job Creation Potential (JCP), differentiated between types of jobs created (i.e., direct and indirect), according to the origin of jobs: in the foreground system or in the background system, apart from

the worker level (high, medium or low) and gender, as further derived from the work of Pillain et al. (2019).

- ii) Occupational Health and Safety (OHS) by means of an Occupational Exposure Limits (OELs) indicator.
- iii) Identification of novel Characterization Factors (CFs) for chemical compounds based on both USEtox and ProScale.

By further improving and incorporating these indicators/aspects into the social assessment, the aim is to help address some of the methodological challenges previously identified and provide a more integrated assessment of the sustainability of the bio-based sectors. In this sense, these quantitative indicators cover some of the overlooked social aspects (e.g., job creation) and target specific stakeholders within the bioeconomy sectors, such as workers exposed to certain chemicals, which are not entirely covered in the Product Environmental Footprint (PEF) methodology.

2.3.1 Job creation potential

The JCP is a social indicator that quantifies the total number of jobs that a product system can generate through the supply chain. In this sense, it represents the aggregation of jobs created in the foreground system and those created by the background system, thus following a cradle-to-grave perspective. Jobs created in foreground systems refer to those required for the operation of a company (i.e., employees directly hired), while jobs created in background systems are those generated by suppliers to support the project. In both cases, the calculation of jobs relies on accounting the Working Hours (WH) associated. For the foreground system, CALIMERO has developed a specific approach, where the required WH are divided by the Full-Time Equivalent (FTE), e.g., at country level, which represents the number of hours a full-time employee works for an organization in a specific time horizon (e.g., one year). WH should be provided directly from the foreground system under assessment (preferably in the form of primary data), while FTE information can be obtained from official statistics, such as those from the Organization for Economic Co-operation and Development (OECD). On the other hand, the methodology developed by Pillain et al. (2019) is used as reference to quantify the jobs of the background system, which includes the process of transforming the LCI into WH terms doing a job coefficients selection, as well as the consideration of the FTE factors. A clear difference with respect to the methodology proposed in CALIMERO is that all steps are referred to the FU. In addition, once it is obtained the total number of potential jobs created (from the foreground and background system) it is possible to upscale this value (referred to the FU selected) by applying a Scaling Factor (SF) in relation to a contextualized situation, such as time period or region (e.g., a year or one country).

This methodology has the advantage of using the same inventory information as the LCA, resulting in significant time and resource savings. Below is a detailed step-by-step description of the procedure to be followed, broken down by foreground and background lifecycle jobs, where the total JCP number is the sum of both (**Figure 2**). A more detailed elaboration of each step can be consulted in *Annex A. Job Creation Potential calculator tool*, which also facilitates the task of estimating the JCP.

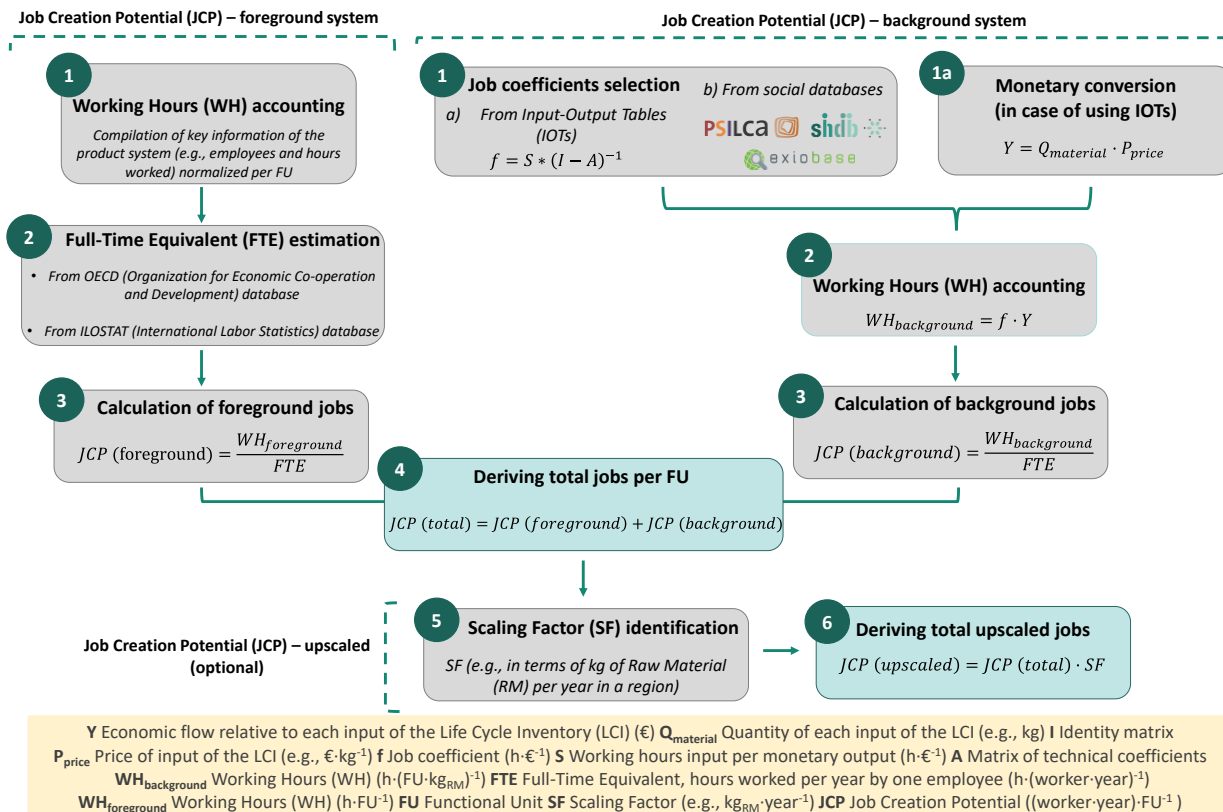


Figure 2. Overview of the methodological steps for determining the job creation potential, partially based on Pillain et al. (2019).

JCP – foreground system / Step 1. Working Hours (WH) accounting

The first step in estimating the potential jobs created is to retrieve or/and calculate the total number of WH for the foreground system under consideration. To do this, it is necessary to collect key information, such as the total number of hours worked, all normalized to the selected FU.

JCP – foreground system / Step 2. Full-Time Equivalent (FTE) estimation

The FTE represents the total number of hours worked per year by an employee. It is important to mention that the FTE varies among else by country, which allows for the identification of jobs created by the acquisition of the different supply chain inputs in their respective countries of origin. These can be obtained directly from the OECD database¹, although some lack of information exists for non-OECD countries. For these non-OECD countries, assumptions can be made based on ILOSTAT (International Labor Statistics), which provides average weekly hours worked per employee. Consequently, these unit can be transformed into annual terms by taking into consideration the number of working weeks per year (at global scale or relativized per country). An example is provided in **Equation 1**.

$$FTE_{\text{non-OECD country}} = WHE \cdot WWY \quad (\text{Equation 1})$$

Where:

$FTE_{\text{non-OECD country}}$: Total number of hours worked per year by one employee at country level relative to a one non-OECD country (h·(worker·year)⁻¹)

WHE : Weekly hours worked per employee relative to a one non-OECD country (h·(worker·week)⁻¹)

WWY : Working weeks per year, this value can be provided relative to a one non-OECD country or

¹ OECD Data Explorer • Average annual hours actually worked per worker

at global scale in case of missing information (week·year⁻¹)

JCP – foreground system / Step 3. Calculation of foreground jobs

Once the WH are accounted for and the FTE value is obtained, the foreground jobs are obtained by applying **Equation 2**.

$$JCP (foreground) = \frac{WH_{foreground}}{FTE} \quad (\text{Equation 2})$$

Where:

JCP (foreground): Number of potential foreground job positions created ((worker·year)·FU⁻¹)

WH_{foreground}: Total number of hours worked (foreground) normalized per FU (h·FU⁻¹)

FTE: Total number of hours worked per year by one employee at country level (h·(worker·year)⁻¹)

JCP – background system / Step 1. Job coefficients selection

In this step, it is necessary to estimate the direct and indirect WH required to produce one monetary unit for each economic sector/process linked through inventory flows. These values are known as job coefficients (f), and can be calculated manually using IOTs or obtained directly from databases. An example of manual calculation is illustrated in the *Appendix A. Job coefficients (f) estimation* for a Spanish context in 2018.

To clarify, direct WH refers to the direct induced jobs, which are the positions filled by employees paid by a supplier and created to provide services. Conversely, indirect WH account from jobs created at a supplier's supplier to develop a direct input (i.e., indirect induced jobs) (Garrabé, 2017).

- **From IOTs**

a. Calculation of the direct coefficients of the volume of working hours

This initial stage “a” involves constructing a matrix (S) that incorporates the direct WH associated with the economic sector identified in the IOTs (K_j) and the monetary production of this economic sector (X_j) (**Equation 3**). If information on direct WH is not available, it can be estimated from the number of workers and the FTE.

$$S_j = \frac{K_j}{X_j} \quad (\text{Equation 3})$$

Where:

S_j: hours worked per monetary unit in an economic sector (j) (h·€⁻¹), an element of matrix S

K_j: Amount of direct WH for an economic sector (j) (h)

X_j: Total quantity of monetary output per economic sector (j) (€)

b. Calculation of the technical coefficients

In stage “b”, a commonly already pre-executed step for IOTs, it is necessary to calculate the technical coefficients using **Equation 4**, which will be used to determine the induced indirect effects on hours worked in the whole economy (i.e., the effects on indirect employment) in the following stage “c”.

$$a_{ij} = \frac{X_{ij}}{X_j} \quad (\text{Equation 4})$$

Where:

a_{ij}: Technical coefficient of an economic sector (i) by total economic output of another economic sector (j), an element of matrix A (matrix of technical coefficients)

X_{ij}: Quantity of monetary units from one economic sector (i) necessary to another economic sector (j) (€)

X_j : Total quantity of monetary output per economic sector j (€)

c. Calculation of the total induced working hours (direct and indirect)

The directly and indirectly induced WH associated with each economic sector in the IOTs is then calculated by applying the inverse matrix model of Leontief, as used in common LCI matrix calculations (Crawford et al., 2018) (**Equation 5**):

$$f = S \cdot (I - A)^{-1} \quad (\text{Equation 5})$$

Where:

- f: Direct and indirect WH required to produce one monetary unit relative to a specific economic sector ($\text{h} \cdot \text{€}^{-1}$)
- S: Matrix of hours worked per monetary unit in an economic sector ($\text{h} \cdot \text{€}^{-1}$)
- I: Identity matrix
- A: Matrix of technical coefficients

- **From databases**

The WH required to produce one monetary unit can be directly obtained from specific databases like SHDB, as proposed by Pillain et al. (2019), but also from PSILCA or EXIOBASE. More precisely, these databases already have pre-collected data for step 1a (monetary conversion), apart from matrixes A and S. The only thing that is needed is to run the inversion using **Equation 5**. For instance, from SHDB and PSILCA one can thus derive coefficients that indicate the direct and indirect WH necessary to generate one monetary output (in terms of United States Dollars) in each economic sector (Pillain et al., 2019). In this context, PSILCA has traditionally utilized WH as an activity variable —i.e., as a metric for evaluating an activity within a process— and has applied it to quantify social indicators. In version 3, an alternative approach is introduced, where results are no longer quantified using WH as the activity variable, instead, the original value of the indicators is used directly (e.g., % child labor) (Springer et al., 2024). In PSILCA, WH are included in the form of “direct hours” (time spent carrying out the tasks and duties of a job), “related hours” (time spent maintaining, facilitating or enhancing productive activities), “downtime” (time when a worker cannot work due to machinery or process breakdown, accident, lack of supplies or power) and “resting time” (time spent in short periods of rest, relief, or refreshment, including tea, coffee or prayer breaks) (Maister et al., 2020). Lastly, EXIOBASE tracks socioeconomic impacts through total and vulnerable employment, considering both the number of persons and hours involved. These indicators are further disaggregated by gender and skill levels (high-, medium-, and low-skilled work), aligning with the International Standard Classification of Occupations (Stadler et al., 2018). This enables the calculation of additional indicators of labor efficiency and work quality, such as forced labor and vulnerable employment (Wood et al., 2014).

JCP – background system / Step 1a. Monetary conversion (in case of using IOTs)

In case of using monetary IOTs, it is required to perform this additional step in order to transform the LCI from service (e.g., transport), physical or energy units (Q_{material}) to monetary terms using the price associated to each input (P_{price}), thus obtaining the economic flow (Y) (**Equation 6**). During this step, it is important to note that the inventory shall be divided by the FU considered in the product system.

$$Y = Q_{\text{material}} \cdot P_{\text{price}} \quad (\text{Equation 6})$$

Where:

- Y: Economic flow relative to each input of the LCI ($\text{€} \cdot \text{FU}^{-1}$)
- Q_{material} : Quantity of each input of the LCI per FU ($\text{kg} \cdot \text{FU}^{-1}$, $\text{kWh} \cdot \text{FU}^{-1} \dots$)
- P_{price} : Price of each input of the LCI (e.g., $\text{€} \cdot \text{kg}^{-1}$, $\text{€} \cdot \text{kWh}^{-1} \dots$)

JCP – background / Step 2. Working hours accounting

To determine the total WH relative to the upstream life cycle stages ($WH_{background}$, $h \cdot FU^{-1}$), **Equation 7** is used. As it was already mentioned, “f” represents the combined number of direct and indirect WH necessary to produce a monetary output in each economic sector, and “Y” denotes the amount of economic flow generated by each process of the LCI.

$$WH_{background} = f \cdot Y \quad (\text{Equation 7})$$

JCP – background system / Step 3. Calculation of background jobs

Once the WH are accounted for and the FTE value is obtained, the background jobs are obtained by applying **Equation 8**.

$$JCP(\text{background}) = \frac{WH_{background}}{FTE} \quad (\text{Equation 8})$$

Where:

JCP (background): Number of potential background job positions created ($(\text{worker-year}) \cdot FU^{-1}$)

$WH_{background}$: Total number of hours worked (background) normalized per FU ($h \cdot FU^{-1}$)

FTE: Total number of hours worked per year by one employee at country level ($h \cdot (\text{worker-year})^{-1}$)

Additionally, by applying the ratio of direct to indirect jobs from statistics for each sector, it is possible to distinguish between direct and indirect employment. To that end, the OECD database can be used.

JCP – foreground and background systems / Step 4. Deriving total jobs per FU

The total number of jobs per FU are obtained by summing both the JCP from the foreground system and the JCP from the background system (see **Equation 9**).

$$JCP(\text{total}) = JCP(\text{foreground}) + JCP(\text{background}) \quad (\text{Equation 9})$$

Where:

JCP (total): Number of potential job positions created ($(\text{worker-year}) \cdot FU^{-1}$)

JCP (foreground): Number of potential foreground job positions created ($(\text{worker-year}) \cdot FU^{-1}$)

JCP (background): Number of potential background job positions created ($(\text{worker-year}) \cdot FU^{-1}$)

JCP – upscaled (optional) / Step 5. Scaling Factor (SF) identification

In this step, a specific SF has to be identified. In this regard, as an example, the amount of the main Raw Material (RM) entering the system can be used as a reference for calculating this factor. The SF is determined by dividing the potential availability of RM within a specific context —both in terms of time and location (e.g., the RM available over the course of one year in Spain)— by the amount required to produce the FU. As a result, the unit of the Scaling Factor will be a “FU scaled”.

JCP – upscaled (optional) / Step 6. Deriving total upscaled jobs

Finally, once the WH of both the foreground and background systems are obtained per FU, they can be further upscaled using the SF identified, by applying **Equation 10**.

$$JCP(\text{upscaled}) = JCP(\text{total}) \cdot SF \quad (\text{Equation 10})$$

Where:

JCP (upscaled): Number of upscaled job positions created (e.g., $\text{worker} \cdot \text{kg}_{\text{RM}}^{-1}$)

JCP (total): Number of potential foreground and background job positions created

((worker·year)·FU⁻¹)

SF: Factor used to scale up the total number of potential jobs to a certain extent in relation to a contextualized situation, such as time period or region (e.g., total availability of the main RM used in the product system per year in mass terms - FU scaled factor)

2.1.1.1 Data requirements and limitations of the job creation potential methodology

Regarding the data requirements for conducting the JCP methodology, **Table 3** summarizes and provide details about the sources from which information can be obtained, whether directly from the producers or social databases (e.g., SHDB) and statistics portals, such as the OECD or Eurostat.

Table 3. Overview of data requirements for estimating the Job Creation Potential.

JCP (foreground)			
Steps	Data	Source	
Step 1. Working Hours (WH) accounting	Number of Working Hours (WH) of the product system from the Life Cycle Inventory (LCI)	Primary data and secondary data	
Step 2. Full-Time Equivalent (FTE) estimation	FTE	Literature and databases (e.g., OECD or ISOSTAT)	
JCP (background)			
Steps	Data	Source	
Step 1. Job coefficients selection	Using IOTs	Workers per sector	Literature and databases (e.g., OECD)
		IOTs	Literature and databases (e.g., OECD)
	Using databases	Induced WH per sector (using Equation 5)	Social databases (e.g., SHDB, PSILCA or EXIOBASE)
Step 1a. Monetary conversion (in case of using IOTs)	Foreground inventory	Primary and secondary data	
	Prices of each inventory input/output	Primary data or from literature and databases (e.g., Eurostat)	
JCP (upscaled)			
Steps	Data	Source	
Step 5. Scaling Factor (SF) identification	SF	Primary and secondary data	

In terms of methodological limitations, it is of paramount importance to note that there is a general restriction of calculating foreground and background systems separately and then adding afterwards, namely it overlooks feedback loops between both of them (if they occur). For example, if the foreground system produces electricity that is used in the background system to generate a product that is indirectly again used in the foreground system. If feedback loops occur, the foreground processes should be taken up in an overall A-matrix that represents the full life cycle before applying the matrix inversion (as done in **Equation 5**). Moreover, even for feedback loops in the foreground system, one should take care in considering loop effects, e.g., by using matrix inverse calculations. Likewise, as previously mentioned, job creation can be quantified using various methods, but not all effects are consistently documented in studies. In this sense, secondary effects, such as the displacement of jobs in the conventional sector by the emergence of new bio-based processes, are often overlooked, thereby neglecting a significant indirect impact.

2.1.1.2 Advancements of the job creation potential methodology

Based on the methodology previously presented in **Section 2.3.1**, one of the CALIMERO partners (LIST) is implementing a number of refinements focusing on two different topics: (i) regionalized FTE for value chain calculations, and (ii) skill and gender differentiation. Both are described in more detail below. It is important to note, however, that these refinements are still under development, so they are not included in *Annex A. Job Creation Potential calculator tool*.

- **Regionalized Full-Time Equivalents for the value chain calculations**

In the approach of Pillain et al. (2019) and also that of the previous section, the JCP from the upstream life cycle stages is estimated by dividing the total number of WH by the FTE corresponding to the location of the foreground system, as shown in Step 3 of **Figure 2**. However, it is interesting to include regionalized FTEs already in Step 1 (see **Figure 2**) before calculating the technical coefficient (f). The idea is to take into account the number of full-time hours worked in each country considered in the background system and thus obtain a more specific FTE value, since it is regionalized per country. This would require a first calculation of the number of jobs per monetary unit per sector using **Equation 11**:

$$J_j = \frac{S_j}{FTE_j} \quad (\text{Equation 11})$$

Where:

- J: Matrix of number of jobs per monetary unit in an economic sector j ((worker·year)·€⁻¹)
- FTE: Matrix with hours worked per year per worker in sector j (h·(worker·year)⁻¹)
- S: Matrix of hours worked per monetary unit in sector j (h·€⁻¹)

Subsequently, **Equation 5** would be replaced by **Equation 12**:

$$f' = J \cdot (I - A)^{-1} \quad (\text{Equation 12})$$

Where:

- f' : Direct and indirect induced jobs required to produce one monetary unit for each analyzed economic sector j (worker·€⁻¹)
- J: Vector of number of jobs per monetary unit in an economic sector j ((worker·year)·€⁻¹)
- I: Identity matrix
- A: Technical coefficients matrix

Following the same logic as in **Equation 7**, jobs are estimated by applying **Equation 13**. As a last step, **Equation 8** does not need to be divided by the FTE, as the unit is already in jobs.

$$Jobs_{LCI} = f' \cdot Y \quad (\text{Equation 13})$$

Where:

- Jobs_{LCI}: Number of job positions created from the LCI ((worker·year)·FU⁻¹)
- f' : Direct and indirect induced jobs required to produce one monetary unit for each analyzed economic sector j ((worker·year)·€⁻¹)
- Y: Amount of economic flow generated by each process of the LCI (€)

Concerning the data to be used for the FTE per sector, it is recommended to use OECD as a reference (as specified in **Section 2.3.1**, see Step 5), although information on FTEs per sector for each country is not available, so country level data should be used instead. In terms of social databases, while EXIOBASE already provides total employment by sector, PSILCA database provides only WH. Therefore, this methodological refinement should be applied when using PSILCA WH. However, EXIOBASE values on total employment are not full-time equivalent job amounts, but number of persons in work (Stadler et al., 2018) (regardless of part-time

or full-time). Hence, the calculation of FTE job amounts is still a separate outcome when applying EXIOBASE.

- **Skill level and gender differentiation**

Another refinement of the presented methodology is to include a differentiation of the jobs created by skill level and gender. Among the labor accounts contained in EXIOBASE, total employment, WH and vulnerable employment are classified into the following six categories: low-, medium- or high-skilled particularized by male or female.

In this case, the vector J (see **Equation 12**) expands to a matrix to contain these different job categories. The estimation of the direct and indirect induced jobs to produce one unit of process unit for each assessed economic sector is performed in the same way as in **Equation 12**, followed by **Equation 13**. Regarding its estimation, LIST will formulate the corresponding code in Python for obtaining the results of the application.

2.3.2 Occupational Exposure Limits indicator

In one deliverable of the CALIMERO project (D2.4 - “Key levers for improvement of sustainability assessment methodology”), assessment of indoor health impacts was listed as one of the gaps in the sustainability assessment for the woodworking sector, and Occupational Exposure Limits (OELs) for relevant chemicals were mentioned for this sector. However, OELs in sustainability assessment are not relevant only for the woodworking sector, but also for other (bio)economy sectors. In the methodological sheets for S-LCA (UNEP et al., 2021), an indicator related to chemical exposure is listed as “preventive measures and emergency protocols exist regarding pesticide and chemical exposure”, although we see a need to suggest a more comprehensive indicator covering management, compliance and OELs.

Table 4. Generic reference scale provided by UNEP et al. (2021), covering the definition of the scores +2 to -2.

Scale level	Description
+2	Ideal performance. Best in class
+1	Beyond compliance
0	Compliance with local and international laws and/or basic societal expectations
-1	Slightly below compliance level
-2	Starkly below compliance level

Table 5. Risk assessment scale for “risk that workers suffer non-fatal accidents” indicator for subcategory “health & safety” for the stakeholder category “worker” in Product Social Impact Life Cycle Assessment (PSILCA) database (Maister et al., 2020).

Indicator value y , # per 100,000 employees	Risk level
$0 \leq y < 750$	Very low risk
$750 \leq y < 1,500$	Low risk
$1,500 \leq y < 2,250$	Medium risk
$2,250 \leq y < 3,000$	High risk
$3,000 \leq y$	Very high risk

In this section, we focus on suggesting an OELs indicator and how to implement it in site-specific S-LCA studies. In S-LCA, for the impact assessment phase, RS or IP approaches can be used. Most used approach so far has been RS approach, on which we also focus in this section. Using an RS, social performance or social

risk of a product can be assessed. RS approaches are ordinal, typically with 1 to 5 levels, and can be either ascending (e.g., from negative to positive performance) or descending. The generic RS for the definition of scales given in UNEP (2020) is shown in **Table 4**.

Table 6. Reference scale for health & safety impact subcategory for the stakeholder category “worker” (Ardolino et al., 2023).

Scale level	Description
+2	There are no risks for workers of the plants of the processes under analysis to be exposed to accidents/damages for health and safety as well as to carry out strenuous activities
+1	There is a low risk for workers of the plants of the processes under analysis to be exposed to accidents/damages for health and safety as well as to carry out strenuous activities
0	There is not a shared position of the experts or there are not enough data available
-1	There is a medium risk for workers of the plants of the processes under analysis to be exposed to accidents/damages for health and safety as well as to carry out strenuous activities
-2	There is a very high risk for workers of the plants of the processes under analysis to be exposed to accidents/damages for health and safety as well as to carry out strenuous activities

Table 7. Occupational health and safety reference scale for the “worker” stakeholder category in (Goedkoop et al., 2020).

Scale level	Description	Performance indicators
+2	The company is best in class compared to its peers on OHS performance	<ul style="list-style-type: none"> • Credible statistics show the OHS performance is best in class compared to its peers in the same sector and region, and this performance has improved over at least 3 years • Credible statements from Non-Governmental Organizations (NGOs), unions and workers that confirm this
+1	The company has a management system in place to proactively and continuously improve the working culture, beyond an acceptable level and can show tangible results of these efforts	<ul style="list-style-type: none"> • Documents that provide a credible description of management system to promote continuous improvement of health and safety and the results of these efforts • Credible statements from NGOs, unions and workers that confirm this
0	Working conditions and working culture are adequately protecting OHS, which includes that equipment, the use of personal protection equipment, the prevention of harassment are conforming to the state of the art regarding safety and exposure	<ul style="list-style-type: none"> • Documents like audits that show compliance with National standards, see Global ILO LEGOSH database • Documents that show certification schemes/standards on health and safety, audits
-1	There has been a neglect in the working conditions (culture) regarding the maintenance and promotion of OHS, which results in high accident rates and deteriorating health conditions of workers, but the company or facility has developed a corrective action plan with clear timeline for completion	<ul style="list-style-type: none"> • While the company is in an area where this situation often occurs according to statistics, there is evidence that the company has started to address the situation with a clearly defined timeline • There are incidents of complaints, lawsuits and other signals but they have been significantly reduced during the last 3 years
-2	There is a neglect in the working conditions (culture) regarding the maintenance and promotion of OHS, which results in high accident rates and deteriorating health conditions of workers	<ul style="list-style-type: none"> • Complaints, lawsuits and other signals • Absence of positive information, while the company is in an area, where the risk of bad OHS situations often occurs according to generic statistics

In an RS, in general but here focusing on OHS, one indicator can be the focus as in the social databases risk scales (**Table 5**) or as in the health and safety RS in the work of Ardolino et al. (2023) (see **Table 6**) or several indicators can be covered in a RS as in Goedkoop et al. (2020) in **Table 7**. The indicators can be qualitative like “presence of a formal policy concerning health and safety” or quantitative like “number/percentage of injuries or fatal accidents in the organization by job qualification inside the company” (UNEP, 2021) or a mix of both indicators can be used in RS approaches covering multiple indicators.

Therefore, based on the above, in the context of the CALIMERO project, an (additional) indicator related to exposure limits and its three levels of assessment has been developed. This additional indicator aims to target OELs to chemicals and the management thereof. The suggested indicator and its three levels (A is the best followed by B and C) are given below.

Level A. Work to eliminate risk (i.e., remove exposure or the culprit chemical) is present.

Level B. Efforts to implement measures that minimize risk for exposure in the work environment are present.

Level C. Prevalent chemical health risks in the work environment are monitored and new risks are systemically identified. In cases where OELs values exist, measurements are carried out and the work environment is managed so that limit values are complied with.

The following questions can be used to evaluate the indicator and its levels. The level each question related to is given in parentheses following the questions:

1. How does the company monitor the risk for exposure to chemicals in the work environment? (C)
2. Are there specific protocols or procedures established to handle and control chemical exposures of workers? (C)
3. Are there routines to identify changes in chemical use? (C)
4. Is there exposure to chemicals that have an OEL value? (C)
5. How often does the company carry out work environment measurements to control and monitor exposure with regard to limit values? (C)
6. What preventive measures are used to manage exposure risk? (B)
7. Do the staff use any Personal Protective Equipment (PPE)? (B)
8. What type of chemical management work is conducted within the company? (A)
9. Are you working to reduce the use of chemicals? (A)

The OEL indicator can be used as an additional information in health and safety RS approaches where indicators like “presence of a formal policy concerning health and safety” and “appropriate work equipment and training” are used or it can be used as a stand-alone indicator where needed. In the S-LCA methodology it is not possible to have standardized RS approaches applicable to all sectors and all locations. For example, in the methodological sheets (UNEP, 2021) for all subcategories, indicators that can be used to in RS approaches are listed, but no generic RS are suggested. Following this approach, the suggested indicator, its levels and the relation of levels to RS scores are given, although an RS is not suggested since that needs to be developed and tailored for the relevant case. Where relevant, the RS for “health & safety” covering OEL indicator, needs

to be developed for each case study in dialogue with stakeholders including specialists.

2.3.3 Novel characterization factors for chemical compounds from USEtox

In the context of OHS, one of the CALIMERO partners (LIST), further advanced toxicity characterization for chemicals. Chemicals in the environment can pose significant risks to human health, particularly to workers who may be exposed to toxic substances during the life cycle of products, including their production, use, and disposal (Johnston and Cushing, 2020). As Occupational Health and Safety (OHS) aims to promote and maintain the highest degree of physical, mental, and social well-being of workers in all occupations (Bondebjerg et al., 2023), chemical toxicity could be one of the key aspects for OHS. This task focuses on human toxicity as an indicator for OHS.

In LCA, impact is assessed by multiplying among else emission amounts of the product system by pre-calculated characterization factors (CF, expressing impact per emission amount) in life cycle impact assessment. For toxicity, USEtox has been widely used and viewed as consensus life cycle impact assessment method, with derived CFs, to assess human health and ecotoxicity within LCA (Jolliet et al., 2017). Developed under the auspices of the UNEP/SETAC Life Cycle Initiative, USEtox is a transparent method and provides CFs for 3104 chemicals, 2526 of which are for ecotoxicity and 949 of which are for human toxicity (Fantke et al., 2017). Differentiated by compartments and sub-compartment, in total 15 types of CFs are provided for each of these chemicals. With regard to human health, USEtox provides seven sub-compartment specific and human-related CFs (emissions to household indoor air, industry indoor air, urban air, continent rural air, continent freshwater, continent seawater, continent natural soil, and continent agricultural soil).

A recent development of Environmental Footprint (EF v3), based on the USEtox method, expanded the chemical coverage to 6549 chemicals by extending the data sources for CF calculation (Sala et al., 2022). Even though with the significant extension on the CF availability, the provided CFs are still not enough to cover the whole range of chemicals available on the global market (von Borries et al., 2023; Wu et al., 2022).

In this project, 99 unique chemicals (**Figure 3**) were of interest by partners to obtain (new) CFs as they were missing or could not be directly obtained by the partners. After LIST looked up these chemicals in the recent EF v3 database, there remained 49 chemicals with missing human-related toxicity CFs and 38 with missing ecotoxicity-related CFs. Using USEtox or EF, calculating CFs for these chemicals requires collecting various data concerning chemical properties to calculate factors related to fate, exposure, and effect. However, some of these data are not always available since they conventionally come from experimental tests that are cost- and time-consuming, confidential or non-transparent, and that could face legislation restrictions for specific in-vivo tests on animals. To address this issue, LIST adopted machine learning (ML) techniques to predict the missing CFs.

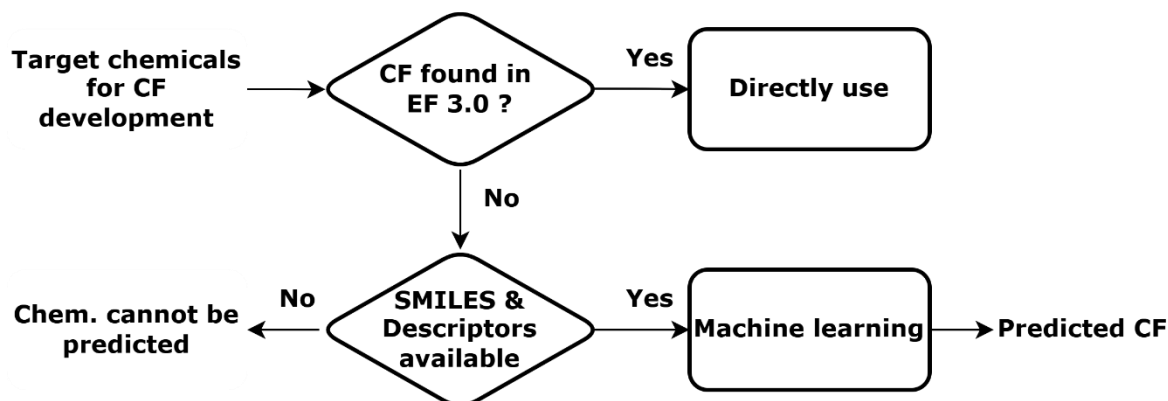


Figure 3. Workflow to collect or predict characterization factors.

The aim of this work is to derive these missing CFs using machine learning aligned with EF v3 based on chemical SMILES (Simplified Molecular Input Line Entry System) strings and associated descriptors. In this deliverable, we focus on the assessment of two human-health related CFs for indoor air emission, i.e., CFs for emissions to household and industrial indoor air. The other ones are presented in D3.1 on Biodiversity. Note that there remain 10 chemicals (see results) that were of interest by partners do not have SMILES sting thus could not use our model to predict CFS.

2.3.3.1 Method to develop characterization factors

The flowchart (**Figure 4**) represents a ML pipeline designed to predict chemical CFs for life cycle impact assessment. Overall, the pipeline takes the chemical and its associated CAS number (a unique accession number assigned by the Chemical Abstracts Service) as inputs and provides predicted CFs as outputs. The process is divided into two key phases: training and prediction. Here, we give a short overview of these phases and then describe specific steps in the subsequent sections.

In the training phase, chemicals CAS number and associated CFs of the targeted indicator are collected from EF v3 dataset. Then their SMILES strings are generated, which are used to generate molecular descriptors, capturing their key structural and physicochemical properties. These descriptors serve as the input for ML-models to learn and to predict CFs. For SMILES structures, we established a multi-source retrieval function in Python to automatically extract SMILES from online chemical databases (CAS Common Chemistry, Chemical Identifier Resolver, and PubChem) through web scraping or application programming interface (API). Molecular descriptors were obtained from SMILE labels using RDKit, an open-source library. Additionally, a clustering step is applied to group chemicals that share similar characteristics based on their descriptors, and we check the model performance for each cluster. For human health, the training process is repeated twice to obtain the trained models for two indicators separately (i.e., indoor household air emission and indoor industrial air emission).

In the predicting phase, the CAS number of the new chemical is used to generate its associated SMILES and descriptors, which are then fed into the trained model of corresponding targeted indicator to predict its CF. The prediction process is also repeated twice to predict two CFs (i.e., indoor household air emission and indoor industrial air emission). Simultaneously, the clustering model from the training phase is applied to help us understand which cluster the new chemical is most similar to in the training dataset. By checking the model performance for the assigned cluster during the training step, we could offer additional insights into how the model may perform on this newly introduced chemical.

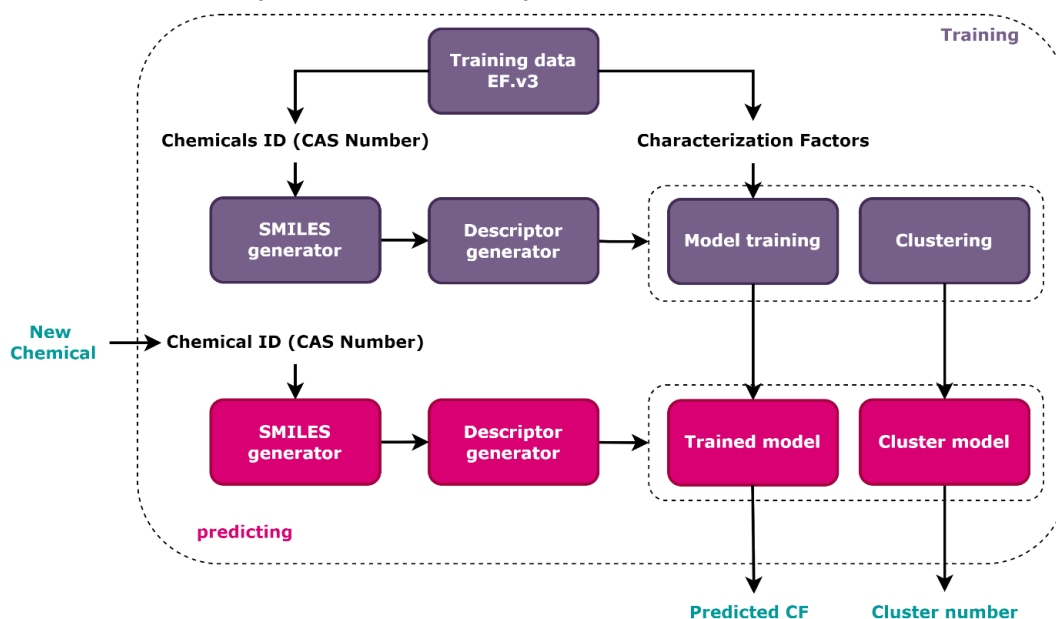


Figure 4. Illustration of the machine learning workflow to predict human toxicity.

2.3.3.2 Data processing

The training data was cleaned by removing chemicals containing no CF for the selected category. Subsequently, we only keep chemicals with descriptors that contain valid values (i.e., no None or NaN). The final dataset contains 3657 observations with one CFs as prediction variables and 198 features as initial predictors for each training.

The dataset CFs present a highly skewed distribution, with most of the values close to zero, which makes it difficult for the model fitting to capture the variance adequately. Therefore, we converted these highly skewed data into log form so that the log-transformed values are more symmetric and closer to a normal distribution.

Note that for human health, USEtox and EF developers manually defined some CFs equal to zero if the calculated CF is too small (e.g., equal to 1E-50). However, these CFs that are manually defined as zero, caused the issue that log transformation could not be performed, as log-transformation requires the values to be non-negative. Therefore, we first constructed a classification model to group the chemicals with CFs equal to zero. This model would be then used to predict chemicals that have zero CFs. Then, for the rest of the chemicals (i.e. for which CFs are higher than zero), we conducted a log-transformation to better capture the variances.

As the descriptors vary widely in scale, we employed a scaling approach (**Equation 14**) to transform each feature individually into values between zero and one. This scaling step assures an equal representation of each feature in the model's learning process.

$$X_{scaled} = \frac{X - X_{min}}{X_{max} - X_{min}} \quad (\text{Equation 14})$$

2.3.3.3 Clustering model

The Gaussian Mixture Model (GMM) was selected as a clustering method. According to Wu et al. (2022), traditional methods—such as range, geometric, distance, and leverage approaches—often lack flexibility or fail to account for the probabilistic nature of cluster boundaries. GMM, in contrast, incorporates probability-oriented and distance-based metrics. This method better captures the multi-dimensional nature of chemical descriptors and enhances the ability to restrict clusters more effectively than conventional methods.

To determine the optimal number of clusters, we used the common approach based on the Bayesian Information Criterion (BIC) indicator, which balances model complexity with goodness of fit. It encourages better fit of the model to the data, but penalizes the model when it is too complicated. Specifically, we compared four covariance types: spherical, tied, diagonal, and full, and for each covariance type we calculated the BIC score for different cluster numbers. The optimal number of clusters is selected when the BIC score is the lowest.

2.3.3.4 Performance measurement

Model performance is measured using the coefficient of determination R^2 , computed using **Equation 15**. This coefficient, ranging between zero to one, is a statistical measure that quantifies how well the model approximates the actual data.

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y}_i)^2} \quad (\text{Equation 15})$$

Where \hat{y}_i are the predicted values, \bar{y}_i is the mean of the observed values, y_i are the actual CFs of the test data set. R^2 represents the proportion of variance accounted for by the model. The higher value (closer to 1) of R^2 denotes the model has better performance and lower value (closer to 0) denotes a worse performance.

Moreover, MSE (Mean Squared Error) was used to provide a more comprehensive evaluation of model performance. MSE measures how close predicted values are to observed values. The smaller MSE value is, the better the model performance is. This work employs MSE to ensure the model performance (see **Equation 16**).

$$MSE = \frac{1}{n} \cdot \sum (y_i - \hat{y}_i)^2 \quad (\text{Equation 16})$$

2.3.3.5 Machine learning models

This work explored two ML models, XGBoost (Extreme Gradient Boosting) and Gaussian Process. XGBoost is a powerful ML algorithm that is widely used because of its speed and efficiency, especially when dealing with large datasets (Chen and Guestrin, 2016). It builds a series of decision trees sequentially, where each new tree aims to improve the predictions by reducing residuals made by previous ones and prevent from overfitting by using regularization.

Gaussian Process is another powerful non-parametric Bayesian approach to modeling complex relationships in data (Rasmussen and Williams, 2008). This approach defines a prior distribution over functions and updates this distribution based on observed data to derive a posterior distribution. The main idea behind it is to assume that the function values for both training and test points, follow a multivariate normal distribution, which allows Gaussian Process to capture uncertainty in predictions. The distribution is defined by a mean vector and a covariance matrix that describes how points are related to each other in terms of similarity (**Equation 17**).

$$\begin{pmatrix} f \\ f_* \end{pmatrix} \sim N \left(\begin{pmatrix} \mu \\ \mu_* \end{pmatrix}, \begin{pmatrix} K & K_* \\ K_*^T & K_{**} \end{pmatrix} \right) \quad (\text{Equation 17})$$

Where the outcome values are constituted with the ones that we have observed (f) and the ones to be identified (f_*). The covariance matrix (K , K_* , K_*^T and K_{**}) measures the similarity between points in training dataset (K), the similarity between training and testing dataset (K_* and its transpose K_*^T), and the similarity between testing dataset (K_{**}). These covariance matrices could be calculated using kernel functions. In this work, it was designed eight types of kernel combinations for the model to compare and model selection.

For both XGBoost and Gaussian Process, the original dataset was split into training (70%) and testing (30%) sets. Three-fold cross-validation was used to choose the best hyperparameter combination from a random search. The best model was then used to predict the test set using the coefficient of determination (R^2) as indicator of performance of the model.

2.3.3.6 Model performance, clustering and predicted characterization factors

We will first discuss the performance as the model before delving into the actual CFs calculated. The prior will define which one to select for deriving the CF of a certain chemical based on the clustering.

Figure 5 displays scatter plots comparing predicted vs. actual values for CF predictions of two CFs (air emissions to household and industrial building) using XGBoost and Gaussian Process models. For XGBoost model (left column), R^2 scores are 0.46 for household emissions and 0.45 for industrial emissions, suggesting a moderate fit, where the predicted values capture a reasonable portion of the variability in CFs. These results of R^2 are within the range of other studies for toxicity prediction (Hou et al., 2020b, 2020a; Kvasnicka et al., 2024).

The Gaussian Process model yields slightly lower scores of 0.4 for both household and industrial emissions, suggesting similar predictive capabilities but has slightly less variance captured than XGBoost.

Despite this, Gaussian Process still could offer advantages in uncertainty quantification, which is a critical factor in toxicity assessments. **Figure 6** illustrates the Gaussian Process model's predicted CFs, with mean predictions and 95% confidence intervals for each chemical prediction. The wide confidence intervals at several points indicate there is a high uncertainty in chemical CF prediction.

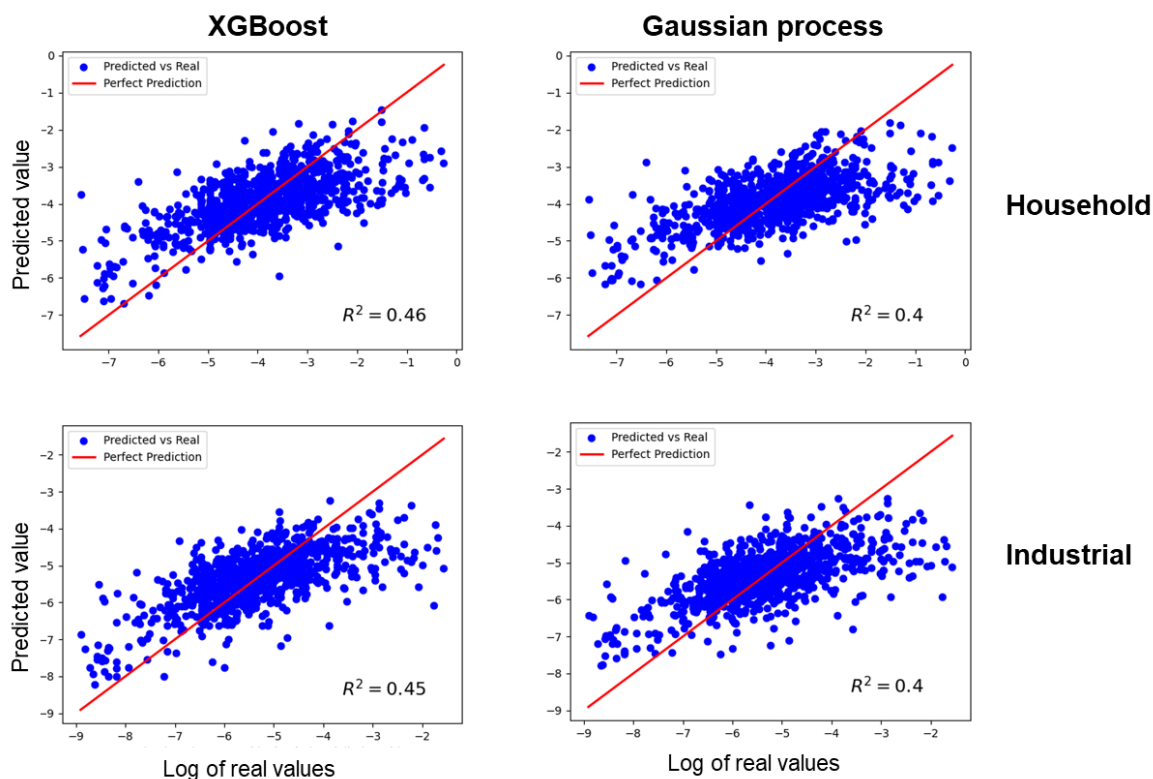


Figure 5. Model performance of XGBoost and Gaussian Process.

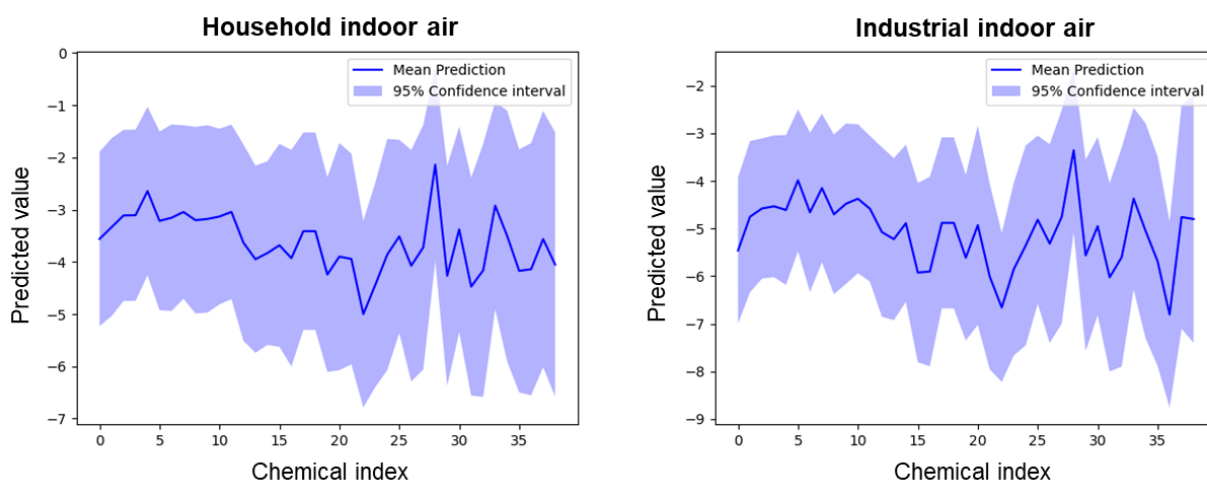


Figure 6. Mean and 95% confidence interval of predicted values through Gaussian Process for the chemicals, listed with their index for visualization (corresponding chemical names are presented in **Error! Reference source not found.**).

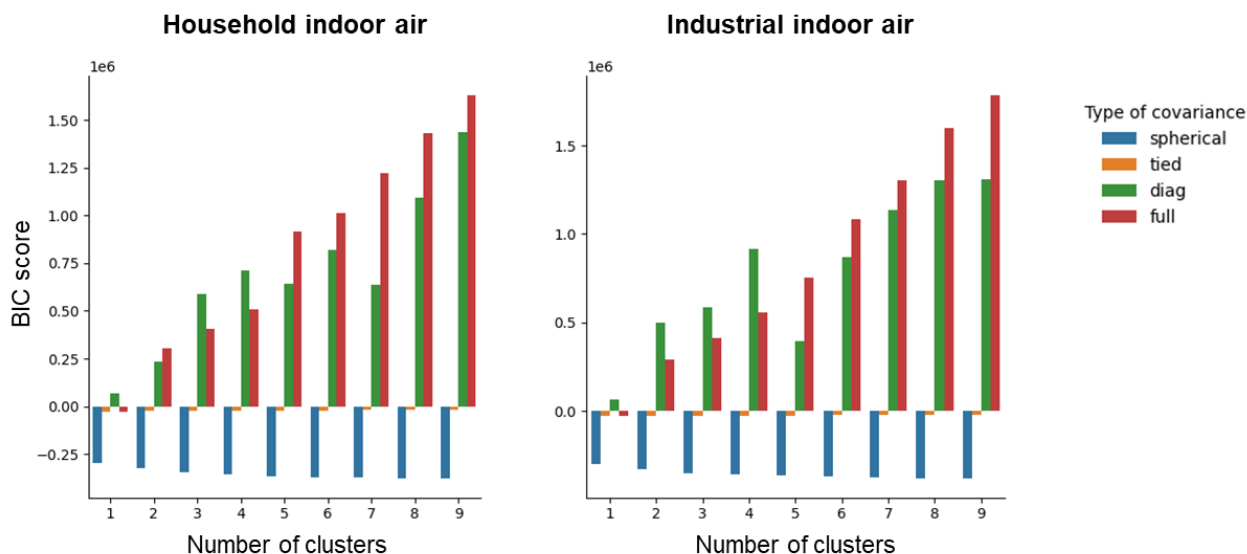


Figure 7. Bayesian Information Criterion score of different cluster number and covariance type.

Figure 7 represents the BIC scores obtained for different numbers of clusters, ranging from 1 to 9, with four covariance types — spherical, tied, diagonal, and full — using GMM. The results show that spherical covariance type consistently yields the lowest BIC scores across all cluster numbers, suggesting that a spherical covariance structure best aligns with the clustering pattern of the training dataset. The BIC scores increase progressively with the number of clusters for other covariance types (tied, diagonal, and full), indicating potential overfitting as model complexity grows. The lowest BIC score appears when spherical covariance type and 9 cluster number are used for the clustering model. This model setting, i.e., spherical variance and 9 cluster, is thus used to cluster new chemicals later in this work (session 3.3).

The performance metrics (R^2 and MSE) for each cluster (**Table 8**) show that both models predict better for some clusters (cluster 0, 4, and 7). However, for some clusters, like cluster 1 and 3 in the industrial compartment, the predictive performance is relatively low for both models, suggesting that these clusters may contain chemicals with unique properties that are difficult to model accurately. This result highlights the variability in model performance across different clusters, suggesting that predictive accuracy depends heavily on cluster-specific characteristics.

Figure 8 compares the predicted CFs for various chemicals through XGBoost and Gaussian Process models. In both plots, both models show a generally similar trend across the chemical indices, indicating that both models recognize similar patterns in the data. For CF prediction on household indoor air emissions (left of **Figure 8**), a significant difference appears on Glucoamylase (chemical 22), which likely stems from the difference between a tree-based model (XGBoost) and kernel-based model (Gaussian Process). The tree-based model could lead to sharper predictions if the model interprets some features as having a strong effect. On the other hand, kernel-based Gaussian Process tends to make more gradual adjustments to predictions.

Though XGBoost in general slightly performs better than Gaussian Process model, Gaussian Process model still outperforms XGBoost in one cluster (**Table 8**). Therefore, to predict CFs for the targeted chemicals, we first assign a cluster number to the target chemicals using the trained GMM, and then select the predicted CFs from the model that have higher R^2 values according to **Table 8**. The recommended CFs from either XGBoost or Gaussian Process are presented in **Table 9**. Finally, in total, 88 chemicals could be found from this task, either collected from EF v3 or predicted through ML model. In this deliverable, only the CFs that are presented through ML models are presented and discussed here.

Table 8. Model performance for each cluster.

Compartment	Cluster_N	R ²		MSE (Mean Squared Error)			
		Gaussian process	XGBoost	Better performance	Gaussian process	XGBoost	Better performance
Household	0	0.41	0.41	XGBoost	1.03	1.02	XGBoost
	1	0.17	0.08	Gaussian	0.98	1.03	Gaussian
	2	0.35	0.21	Gaussian	0.60	0.66	Gaussian
	3	0.31	0.26	Gaussian	0.83	0.85	Gaussian
	4	0.39	0.38	Gaussian	0.85	0.86	Gaussian
	5	0.58	0.65	XGBoost	1.05	0.97	XGBoost
	6	0.47	0.34	Gaussian	0.72	0.80	Gaussian
	7	0.36	0.41	XGBoost	1.15	1.10	XGBoost
	8	0.31	0.17	Gaussian	0.70	0.77	Gaussian
Industrial	0	0.48	0.59	XGBoost	0.98	0.88	XGBoost
	1	0.10	0.08	Gaussian	0.62	0.63	Gaussian
	2	0.39	0.43	XGBoost	0.97	0.94	XGBoost
	3	0.03	0.19	XGBoost	1.36	1.24	XGBoost
	4	0.40	0.37	Gaussian	0.87	0.89	Gaussian
	5	0.28	0.32	XGBoost	0.80	0.78	XGBoost
	6	0.43	0.52	XGBoost	0.88	0.81	XGBoost
	7	0.19	0.21	XGBoost	0.97	0.95	XGBoost
	8	0.18	0.31	XGBoost	0.81	0.75	XGBoost

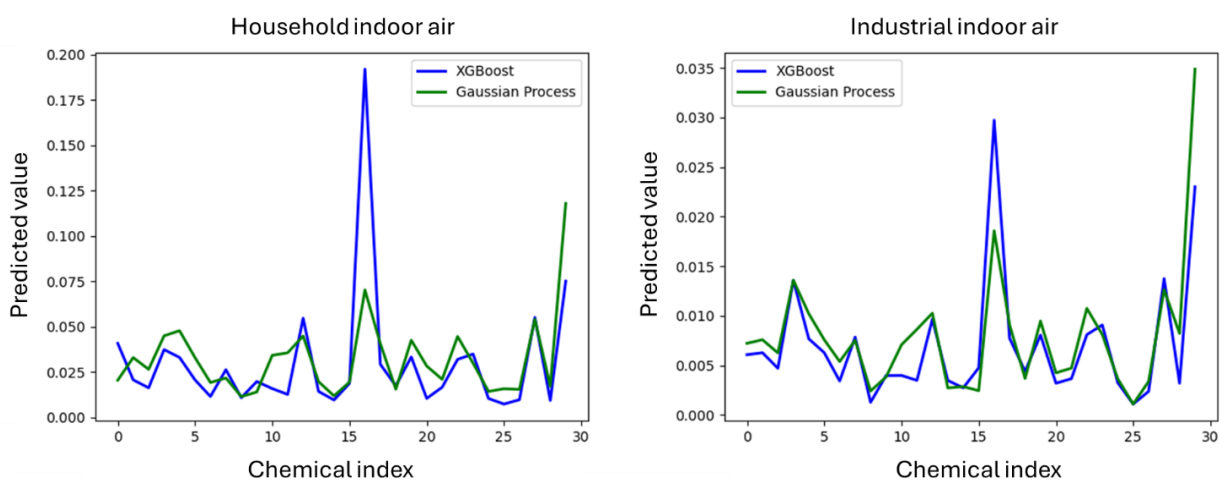


Figure 8. Comparison of predicted values using XGBoost and Gaussian Process.

It should be noted that these CFs represent the impacts of per kg of chemicals that are already emitted to air. Therefore, for conducting LCA, one should also know how much of these chemicals are emitted to indoor air, whether to industrial buildings or household buildings. Such information could be found in literature (e.g., Roos et al., 2019) or databases such as Specific Environmental Release Categories (known as “SpERCs”), which is not the focus of this work.

Table 9. Predicted characterization factors for household indoor air and industrial indoor air (in units of cases per kg of chemical emitted).

Chemical Name	CAS	Indoor air household	Indoor air industry
Calcium chloride	10043-52-4	0.035	0.0073
4,4'-Diisocyanatodiphenylmethane	101-68-8	0.054	0.0126
Nitric oxide	10102-43-9	0.034	0.0061
Ceric sulfate tetrahydrate	10294-42-5	0.021	0.0047
Dipotassium phosphate	7758-11-4	0.011	0.0027
Borax pentahydrate	12179-04-3	0.019	0.0049
Carbon dioxide	124-38-9	0.017	0.0047
Sodium oxide	12401-86-4	0.026	0.0077
Cobalt Molybdenum Alloy	39422-44-1	0.037	0.0136
Sodium tetraborate decahydrate	1303-96-4	0.018	0.0037
Calcium hydroxide	1305-62-0	0.021	0.0078
Potassium hydroxide	1310-58-3	0.030	0.0077
Caustic soda	1310-73-2	0.028	0.0081
Sodium oxide	1313-59-3	0.028	0.0081
Zeolite	1318-02-1	0.024	0.0063
H-Mordenite	1318-02-1	0.024	0.0063
Gypsum	13397-24-5	0.011	0.0034
Polyethylene glycol dimethyl ether	24991-55-7	0.007	0.0016
Methylisothiazolinone	2682-20-4	0.037	0.0091
Tungstic acid	7783-03-1	0.024	0.0048
Sodium Carbonate	497-19-8	0.023	0.0079
Glucose	50-99-7	0.010	0.0013
Platinum	7440-06-4	0.039	0.0135
Cobalt acetate	6147-53-1	0.018	0.0040
Hydroxymethylfurfural (HMF)	67-47-0	0.012	0.0040
Molasses	68476-78-8	0.005	0.0015
Boron	7440-42-8	0.011	0.0032
Hydrochloric acid	7647-01-0	0.011	0.0035
Sodium Chloride	7647-14-5	0.049	0.0097
Phosphoric acid	7664-38-2	0.020	0.0035
Disodium disulphite	7681-57-4	0.010	0.0033
2,6-Bis(2-isocyanato-3-((2-isocyanatophenyl)methyl)benzyl)phenyl isocyanate	85423-11-6	0.010	0.0032
Hexane, 1,6-diisocyanato-	88357-62-4	0.085	0.0230
Sulfur dioxide	7446-09-5	0.025	0.0038
Cellulase	9012-54-8	0.008	0.0011
Kieralon MWF (hostapal MWF, soap)	9043-30-5	0.008	0.0024
(2Z)-2-[(10E)-10-[cyano(isociano)methylidene]-3-(3-methyloxiran-2-yl)-2,7,8-tris(oxiran-2-yl)-4b,9b-dihydroindeno[2,1-a]inden-5-ylidene]-2-isocyanoacetone nitrile		0.013	0.0086
1,1,1-Tris(4-cyanatophenyl)ethane		0.030	0.0064

The remaining 11 chemicals (shown in **Table 10**) cannot be predicted because they don't have SMILES, which is the structure our model relies on to generate descriptors. These represent a diverse group of industrial and biochemical substances, including enzymes, polymers, surfactants, and inorganic compounds. To calculate their toxicity CFs, further study should be conducted, e.g., through searching more databases that have not been covered by EF v3.

Table 10. Chemicals that do not have characterization factors collected or predicted.

Sector	Chemical name	CAS
Biochemical	Fodder yeast	8013-01-2
Biochemical	Amylase	9000-90-2
Biochemical	Lubricating oil	93572-43-1
Biochemical	Glucoamylase	9032-08-0
Textile	Polyaluminium chloride	1327-41-9
Textile	Polyester copolymer	139755-78-5
Textile	Poly(oxy-1,2-ethanediyl), α -hydro- ω -hydroxy- Ethane-1,2-diol, ethoxylated	25322-68-3
Textile	Fatty alcohol ethohylate	68439-49-6
Textile	Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	68411-30-3
Textile	Alcohols, C16-18, ethoxylated	68439-49-6
Textile	Anionic polyacrylamide	9003-0-8

2.3.4 Novel characterization factors for chemical compounds from ProScale

In this project, apart from those CFs identified from USEtox, additional ones were also proposed from ProScale. As a starting point, 90 of the chemicals of interest to the partners of the CALIMERO project were assessed with the aim to calculate its CFs with ProScale for human toxicity with data mainly reported under REACH (Registration, Evaluation, Authorization and Restriction of Chemicals Regulation) and predicted information.

This ProScale methodology is an LCIA methodology that can be used for assessment of toxicity potentials of chemicals in an LCA setting (Lexén et al., 2021). The scope of ProScale covering direct exposure makes it potentially suitable for quantifying chemical exposure related health risks for OHS is one of the key areas of interest of S-LCA and the approach has been briefly testes in this context (Johansson et al., 2023).

This indicator utilizes specific toxicological exposure potential due to direct exposure to hazardous substances rather than a multi-media fate model as in, for instance, USEtox. ProScale is built upon four aggregated parameters: (i) Hazard Factor (HF), (ii) Exposure Concentration Factor (ECF), (iii) Person-Hours Factor (PHF), and (iv) Mass Flow (MF).

These parameters are used to calculate a ProScale score (see **Equation 18**), which can be aggregated for eather a unit process or a product.

$$ProScale\ score = HF \cdot ECF \cdot PHF \cdot MF \quad (\text{Equation 18})$$

CFs in ProScale are derived from the HF, which is in turn derived from hazard phrases (H-phrases), and the OEL or Derived No Effect Level (DNEL) (see **Table 11**), apart from the physical state of the substance

(vapor pressure/dustiness). Other factors are also relevant for the calculation of the final ProScale score but are dependent on the exact process conditions, such as the use or not of protective equipment, local exhaust ventilation and other exposure determinants. The PHF and MF are properties of the process assessed and the product system, and therefore not part of the CF calculation. Details about the algorithms are described in the work conducted by Lexén et al. (2021). For the sake of deriving ProScale score, this section deals with developing HFs for as many as possible of the almost 100 chemicals specific to the CALIMERO project.

Table 11. ProScale hazard class and its derivate H-phases according to GHS/CLP (Globally Harmonized System of Classification and Labelling of Chemicals/Classification, Labelling and Packaging), grouped by exposure route.

ProScale hazard class	H-phrases according to GHS/CLP, grouped by exposure route
E 10,000 - 100,00 (highest hazard)	All routes: H340, H350, H360, H362
D 1,000 - 10,000	Dermal: H310 Inhalation: H330, H334, EUH032 Oral: H300 All routes: H341, H351, H361, H372
C 100 - 1,000	Dermal: H311, H314, H317, H318, EUH070 Inhalation: H331, EUH029, EUH031, EUH071 Oral: H301, H304 All routes: H370, H373
B 10 - 100	Dermal: H312, H315, H319 Inhalation: H332, H335 Oral: H302 All routes: H371
A 1 - 10 (lowest hazard)	Dermal: H313, H316, H320, EUH066 Inhalation: H333, H336 Oral: H303, H305

2.3.4.1 Method for data collection from the European Chemicals Agency's

For the calculations of ProScale CFs, data was extracted mainly from REACH dossiers at the European Chemicals Agency's (ECHA) website. H-phases were collected following the prioritization list in ProScale documentation. However, since the release of ProScale, ECHA has launched the website ECHA CHEM ([ECHA CHEM](#)) for its new public chemical database. Therefore, if a substance also had additional hazard phrases listed in a full, lead dossier at the new website, those were used too. Of the 90 substances, 35 were missing or did not have H-phrases in ECHA's database.

In addition, If OELs were available for the substance in the ProScale spreadsheet those were used. For substances where OELs were missing but systemic DNELs for worker inhalation hazards were available from ECHA, those were used, otherwise the model was run with a default OEL of $1.0 \cdot 10^{-3} \text{ mg} \cdot \text{m}^{-3}$.

For fluids, vapor pressure was generally collected from the REACH Factsheets or the Brief profile at ECHA but some were also extracted from other sources e.g. PubChem, Comptox. For solid substances, an evaluation of its dustiness level is required for a ProScale assessment. In this case, where very only brief information is available about the substances, the precautionary principle was employed. Thus, all substances were assumed to have a high dustiness level except for boric acid, which was described in ECHA to be "nearly dust free". In this specific case, a low dustiness level was selected.

In a complete ProScale assessment the parameters MF, PHF, Process Category, and knowledge of the use of Local Exhaust Ventilation and Respiratory Protection is required. In this case, where the aim is to only calculate CFs, the settings listed **Table 12** were employed.

Table 12. Process specific settings used for the calculation of Characterization Factors (CFs).

Parameter	Setting
MF (Mass Flow)	Empty
PHF (Person-Hours Factor)	Empty
Process Category	PROC 1 – Used in closed process, no likelihood of exposure
Type of setting	Professional
Local Exhaust Ventilation	No
Respiratory Protection	No

2.3.4.2 Prediction and treatment of data for ProScale

For chemicals without H-phrases, ML models can be used to provide predictions for chemicals with clear structure information (i.e., SMILES). These models were developed in the Mistra SafeChem project (Halling, 2024), where H-phrases classification data were extracted from the REACH registration dossiers to train and test the models with graphical neural networks. These models cover all human toxicity H-phrases in the CLP (Classification, Labelling and Packaging) regulation. The conformal prediction framework was used to control prediction uncertainties, and the prediction results were assigned to five different categories with a confidence cut-off of 80%:

- **Positive:** The model predicts that the compound is toxic and should have an H-phrase label regarding the target endpoint. The prediction has at least 80% of confidence.
- **Not available with set confidence level, likely positive:** The model predicts that the compound is likely toxic and should have an H-phrase label regarding the target endpoint. However, the prediction cannot reach 80% of confidence level.
- **Negative:** The model predicts that the compound is non-toxic regarding the target endpoint. The prediction has at least 80% of confidence.
- **Not available with set confidence level, likely negative:** The model predicts that the compound is likely non-toxic regarding the target endpoint. However, the prediction cannot reach 80% of confidence level.
- **Out of domain:** The target chemical is too distanced from the chemicals in the model's training set, and the model cannot assign either label (positive or negative) with confidence to the target compound.

Detailed information about these prediction models can be found on the ProScale website (Zheng, 2024). In this study, the models were able to provide predictions for additionally 11 of the 35 substances that does not have H-phrases classification in REACH dossiers. The result of the predictions for each group of H-phrases are provided and used as in **Table 13**. The outcome of the predictions is grouped by toxicity endpoints according to REACH dossiers, and some endpoints have more than one corresponding H-phrase. For example, "acute oral toxicity" has four corresponding H-phrases (H300, H301, H302 and H303). In such cases, a precautionary approach was taken into account and the most severe H-phrase label was used for calculation.

Following the precautionary principles, all predicted H-phrases were added to the ProScale Excel tool and the H-phrase which gives the highest hazard class according to the ProScale ranking was used to determine the CF. For carbon dioxide (124-38-9) and dimethyl sulfoxide (67-68-5), manual selection of the highest ranked

H-phrase for each group of predicted H-phrases was instead carried out. The selection is based on the same ranking of H-phrases as for all other substances.

Table 13. Interpretation of predicted results.

Prediction result	Interpretation
Positive	Used for calculation
Not available with set confidence level, likely positive	Used for calculation, but with caution
Negative	Not used for calculation
Not available with set confidence level, likely negative	Not used for calculation
Out of domain	Not used for calculation

If the exposure route was not included in the name of the prediction, it was assumed the H-phrases were applicable to all routes, inhalation, dermal, and oral. Lastly, when predicted H-phrases were used only default OELs were utilized, even for substances where an OEL or DNEL was available, apart from this all settings were the same as described in **Table 12**.

2.3.4.3 Results and discussion

In total, it was possible to calculate CFs for 52 substances using H-phrases from the REACH registration dossiers retrieved from ECHA. With the predicted H-phrases it was only possible to calculate 10 CFs due to other missing parameter information, all CFs can be found in **Table 14**. Of the CFs based on H-phrase predictions, six of them are either completely or partly based on predictions that are “likely positive”.

Table 14. ProScale Characterization Factors (CFs). *Substances completely based on “likely positive” H-phrases, **Substances partly based on “likely positive”.

Chemical name	CAS	ProScale CF		
		Inhalation	Dermal	Oral
With H-phrases from ECHA				
Boric acid	10043-35-3	6.23E+00	0.00E+00	0.00E+00
Calcium chloride	10043-52-4	3.16E+00	3.16E+01	0.00E+00
4,4'-Diisocyanatodiphenylmethane	101-68-8	1.00E+04	1.00E+04	1.00E+04
Nitric oxide	10102-43-9	1.00E+04	1.00E+03	0.00E+00
Ceric sulfate tetrahydrate	10294-42-5	0.00E+00	1.00E+03	0.00E+00
Butyric acid	107-92-6	1.76E+01	1.76E+02	1.76E+01
Diisobutyl ketone	108-83-8	1.58E+01	0.00E+00	0.00E+00
Cyclohexane	110-82-7	1.00E+00	1.00E+01	1.00E+02
2-Phenoxyethanol	122-99-6	1.27E+01	1.27E+02	1.27E+01
Flumexol WDN	126-71-6	1.61E+00	1.61E+02	0.00E+00
Boric oxide	1303-86-2	1.00E+05	1.00E+05	1.00E+05
Sodium tetraborate decahydrate	1303-96-4	1.00E+05	1.00E+05	1.00E+05
Calcium hydroxide	1305-62-0	5.08E+01	5.08E+02	0.00E+00
Calcium oxide/Lime/Quicklime	1305-78-8	5.08E+01	5.08E+02	0.00E+00
Potassium hydroxide	1310-58-3	0.00E+00	1.00E+03	1.00E+02
Caustic soda	1310-73-2	0.00E+00	1.00E+03	0.00E+00
Sodium oxide	1313-59-3	0.00E+00	1.00E+03	0.00E+00
Monoethanolamine	141-43-5	3.14E+01	3.14E+02	3.14E+01
Ethyl acetate	141-78-6	1.00E+00	1.00E+01	0.00E+00
Polyethylene glycol dimethyl ether	24991-55-7	1.00E+05	1.00E+05	1.00E+05

Table 15. ProScale Characterization Factors (CFs). *Substances completely based on “likely positive” H-phrases, **Substances partly based on “likely positive”.

Chemical name	CAS	ProScale CF		
		Inhalation	Dermal	Oral
With H-phrases form ECHA				
Methylisothiazolinone	2682-20-4	1.00E+04	1.00E+03	1.00E+03
Sodium Carbonate	497-19-8	1.00E+01	1.00E+02	0.00E+00
Formaldehyde	50-00-0	2.27E+04	2.27E+04	2.27E+04
Toluene diisocyanate/Toluene, 2,4-diisocyanate	584-84-9	1.00E+04	1.00E+03	0.00E+00
Ethylenediaminetetraacetic acid	60-00-4	4.51E+01	0.00E+00	0.00E+00
Cobalt acetate	6147-53-1	1.00E+05	1.00E+05	1.00E+05
Ethanol	64-17-5	1.00E+00	1.00E+01	0.00E+00
Acetic acid	64-19-7	1.97E+00	1.97E+02	0.00E+00
Prestogen FCB	6419-19-8	0.00E+00	1.00E+02	0.00E+00
Hydroxymethylfurfural (HMF)	67-47-0	1.00E+02	1.00E+03	0.00E+00
Methanol	67-56-1	1.00E+02	1.00E+02	1.00E+02
Acetone	67-64-1	1.00E+00	1.00E+01	0.00E+00
Chloroform	67-66-3	3.88E+03	3.88E+03	3.88E+03
Benzenesulfonic acid, C10-13-alkyl derivs., sodium salts	68411-30-3	2.80E+00	2.80E+02	2.80E+01
Butanol	71-36-3	1.00E+01	1.00E+02	1.00E+01
Ethylene	74-85-1	1.00E+01	0.00E+00	0.00E+00
Nickel	7440-02-0	1.00E+04	1.00E+04	1.00E+04
Dichloromethane	75-09-2	1.10E+03	1.10E+03	1.10E+03
Hydrochloric acid	7647-01-0	3.68E+02	3.68E+02	0.00E+00
Phosphoric acid	7664-38-2	4.14E+00	4.14E+02	4.14E+01
Ammonia	7664-41-7	2.34E+02	2.34E+02	0.00E+00
Sulphuric acid	7664-93-9	1.00E+01	1.00E+03	0.00E+00
Sodium hypochlorite	7681-52-9	4.46E+00	4.46E+02	0.00E+00
Disodium disulphite	7681-57-4	1.03E+00	1.03E+02	1.03E+01
Sulphur	7704-34-9	0.00E+00	1.00E+02	0.00E+00
Iron sulfate	7720-78-7	0.00E+00	1.00E+02	1.00E+02
Potassium Permanganate	7722-64-7	8.15E+00	8.15E+02	8.15E+01
Hydrogen peroxide	7722-84-1	4.60E+01	4.60E+02	4.60E+01
Sodium persulfate	7775-27-1	5.38E+03	5.38E+02	5.38E+01
Chlorine	7782-50-5	4.51E+02	4.51E+01	0.00E+00
Diisocyanates	822-06-0	1.00E+04	1.00E+03	0.00E+00
Cellulase	9012-54-8	1.00E+04	0.00E+00	0.00E+00
With predicted H-phrases				
Triethanolamine**	102-71-6	1.00E+05	1.00E+05	1.00E+05
Carbon dioxide	124-38-9	3.33E+03	3.33E+03	3.33E+03
Sodium oxide	12401-86-4	0.00E+00	1.00E+03	0.00E+00
Gypsum**	13397-24-5	1.00E+04	1.00E+04	1.00E+04
(2-methoxymethylethoxy)propanol*	34590-94-8	0.00E+00	1.00E+03	0.00E+00
Urea**	57-13-6	1.00E+05	1.00E+05	1.00E+05
Dimethyl sulfoxide**	67-68-5	1.00E+05	1.00E+05	1.00E+05
Boron	7440-42-8	1.00E+05	1.00E+05	1.00E+05
Sodium Chloride	7647-14-5	0.00E+00	1.00E+03	1.00E+04
Ammonium sulfate*	7783-20-2	0.00E+00	1.00E+03	0.00E+00

For 28 substances no CFs were calculated, see **Table 15** mostly because hazard phrases were missing in the dossier from ECHA or it was not possible to predict them, another reason was missing parameters e.g. vapor pressure. For one of the 11 substances where H-phrases were predicted it was, as described earlier, not possible to calculate CFs due to other missing data.

Table 16. Substances for which no Characterization Factors (CFs) were calculated for ProScale and therefore currently left as data gaps.

Chemical name	CAS	Motivation
Dipotassium phosphate	7758-11-04	Not in ECHA, prediction not possible
Borax pentahydrate	12179-04-3	Unknown physical state
Zinc oxide	1314-13-2	No H-phrase in ECHA, no prediction
Zirconium dioxide	1314-23-4	No H-phrase in ECHA, negative predictions
H-Mordenite	1318-02-1	No H-phrase in ECHA, negative predictions
Zeolite		No distinct SMILES or CAS
Aluminum oxide	1344-28-1	No H-phrase in ECHA, negative predictions
Aluminium hydroxide	21645-51-2	No H-phrase in ECHA, negative predictions
Poly(oxy-1,2-ethanediyl), α -hydro- ω -hydroxy- Ethane-1,2-diol, ethoxylated	25322-68-3	No H-phrase in ECHA, negative predictions
Tungstic acid	7783-03-01	Not in ECHA, prediction not possible
Tris (2,4-ditert-butylphenyl)	31570-04-4	No H-phrase in ECHA, negative predictions
Calcium carbonate	471-34-1	No H-phrase in ECHA, negative predictions
Glucose	50-99-7	No H-phrase in ECHA, negative predictions
Rucholase HCH	56-81-5	No H-phrase in ECHA, negative predictions
Platinum	7440-06-04	Not in ECHA, prediction not possible
Molasses	68476-78-8	Positive prediction, missing vapor pressure
Isotridecanol, ethoxylated/Poly(oxy-1,2-ethanediyl), α -tridecyl- ω -hydroxy-, branched	69011-36-5	No H-phrase in ECHA, negative predictions
Methane	74-82-8	No H-phrase in ECHA, negative predictions
Magnesium sulfate	7487-88-9	No H-phrase in ECHA, negative predictions
Diammonium phosphate	7783-28-0	No H-phrase in ECHA, negative predictions
2,6-Bis(2-isocyanato-3-((2-isocyanatophenyl)methyl)benzyl)phenyl isocyanate	85423-11-6	Missing information
Hexane, 1,6-diisocyanato-	88357-62-4	Missing information
Sulfur dioxide	7446-09-05	Not in ECHA, prediction not possible

Table 17 (cont). Substances for which no Characterization Factors (CFs) were calculated for ProScale and therefore currently left as data gaps.

Chemical name	CAS	Motivation
Octadecane -1-ol ethoxylated	9005-00-9	No H-phrase in ECHA, negative predictions
Glucoamylase	9032-08-0	Unknown physical state
Kieralon MWF (hostapal MWF, soap)	9043-30-5	Missing vapor pressure
1,1,1-Tris(4-cyanatophenyl)ethane		No CAS, no SMILES
(2Z)-2-[(10E)-10-[cyano(isocyano)methylidene]-3-(3-methyloxiran-2-yl)-2,7,8-tris(oxiran-2-yl)-4b,9b-dihydroindeno[2,1-a]inden-5-ylidene]-2-isocyanacetoneitrile		No CAS, no SMILES

3 ECONOMIC EVALUATION OF TARGET BIO-BASED INDUSTRIES

3.1 State-of-the-art

LCC is the economic component of an LCSA (Swarr et al., 2011). The LCC methodology was originated in the United States military department in the 1930s for purely economic purposes, and since then has evolved into three different branches, all aimed at evaluating costs over the life cycle of products and services (Rödger et al., 2018):

- The conventional LCC (cLCC) method focuses solely on the internal costs and benefits borne by a single actor directly involved in the analyzed systems.
- The environmental LCC (eLCC) method extends the cLCC method to include internal costs associated with the life cycle of products or services. Consequently, eLCC follows a multi-stakeholder perspective. It can also be complemented by the inclusion of monetized environmental externalities, commonly referred to as full eLCC (feLCC) (Hoogmartens et al., 2014).
- The societal LCC (sLCC) assesses all life cycle costs that are borne by anyone in the society, therefore including both internal costs from all actors linked to the analyzed system, as well as external costs in the form of both social and environmental externalities.

Unlike the standardized LCA, which evaluates the environmental dimension of sustainability according to ISO 14040 and 14044 standards (ISO, 2006a, 2006b), the LCC methodology lacks global standardization. While cLCC has multiple standards and methodological guidelines (UNE 60300-3-3:2017, BS 3843-3:1992, AS/NZS 4536), these are often industry-specific, targeting sectors like construction (ISO 15686, Davis Langdon Management Consulting, 2007), and fossil fuels (ISO 15663:2021), which can make it difficult to consistently apply LCC in different contexts. The SETAC LCC Working Group and Task Force have established fundamental concepts for eLCC assessment, which are reflected in the work of Hunkeler et al. (2008) and Swarr et al. (2011).

Likewise, the EU has established a methodological basis for promoting the use of feLCC in public procurement processes. In this regard, it is included costs borne by the contracting entity or other users (i.e., acquisition, use such as consumption of energy and other resources, maintenance, and EoL), apart from the cost imputed to environmental externalities which may include the cost of greenhouse gas (GHG) or other pollutant emissions, climate change mitigation costs, among others. All these measures appear collected in

Directives 2014/24/EU² (Article 68), 2014/25/EU³ (Article 83) and 2009/33/EC⁴ (policy measure 2c). However, there are still methodological gaps and a lack of consensus on various aspects across these documents, which requires further efforts towards a more consistent and unified methodology (Bianchi et al., 2020).

The life cycle approach of eLCC makes it a useful tool to evaluate the economic aspect within LCSA. However, it has been criticized for its narrow focus on cost-related economic issues (Gluch and Baumann, 2004; Wood and Hertwich, 2013), without considering other important aspects such as value added and growth. To address this gap, Neugebauer et al. (2016) defined a set of impact categories, including profitability, productivity, business diversity, and long-term investment, to broaden the economic scope of eLCC and align it more closely with LCA, particularly in the LCIA phase, and dubbed it “economic LCA” to differentiate it from eLCC. Yet, based on this work, Arulnathan et al. (2022) proposed a collection of indicators linked to the impact categories to operationalize the new suggested areas within LCC.

In addition to eLCC, other methodologies such as Techno-Economic Assessment (TEA), Total Cost of Ownership (TCO), and Material Flow Cost Accounting (MFCA) are adopted for economic analysis within LCSA, even though they are not directly related to LCT (Bianchi et al., 2020). TCO covers the total costs to be paid by the owner (Wynstra and Hurkens, 2005). However, both TCO and eLCC are often used interchangeably, but it is important to note that while eLCC can take multiple stakeholders into account, TCO only considers the costs from the perspective of the owner, thus following a single stakeholder approach. So, in conclusion, it could be said that TCO would be closer to resemble a cLCC. TEA is known for evaluating both technical and economic performance, usually with a focus on the production phase of the life cycle. TEA can be implemented following the same methodological phases as an LCA (Zimmermann et al., 2022, 2020), making it a complementary tool for a comprehensive analysis of both technical and economic aspects. Regarding MFCA, this is a standardized methodology (ISO 14051:2011) that measures material flows and stocks in both physical and economic terms by using a mass-balance approach (Kauffman and Lee, 2013). Therefore, this tool can provide insights into the efficiency of material use across entire value chains (Bux and Amicarelli, 2022).

Among the three LCC methodologies abovementioned, eLCC is currently the preferred approach for assessing economic issues in LCSAs due to its close alignment with the LCA methodology and compliance with ISO 14040 and 14044 (Hunkeler et al. (2008), Swarr et al. (2011), Hauschild et al. (2018), Bianchi et al. (2020), Arulnathan et al. (2022)), which facilitates consistency and synergies with the assessment of the environmental dimension within the wider framework of LCSA. However, the lack of a stakeholder-specific perspective has been criticized. More precisely, because the (financial) viability of a system depends on the acceptability of financial cost-benefit analysis of the stakeholders involved, the consideration of a life cycle perspective is lacking and should best be complemented with individual cLCC per key stakeholders (Schaubroeck et al., 2019).

The abovementioned drawback, along with some others when conducting an eLCC study, have been proposed to be addressed by following a comprehensive procedure introduced by Bachmann et al. (2024) as part of the ORIENTING project. This includes an alignment with the LCSA methodology, address of both externalities and double counting issues between sustainable dimensions accounting (i.e., LCA, LCC and S-LCA), differentiation between three stakeholder perspectives: (i) manufacturing companies, (ii) consumers and

² Directive 2014/24/EU of the European Parliament and the Council of 26 February 2014 on public procurement and repealing Directive 2004/18/EC.

³ Directive 2014/25/EU on public procurement by entities operating in the water, energy, transport and postal services sector and repealing Directive 2004/17/EC.

⁴ Directive 2009/33/EC of the European Parliament and of the Council on the promotion of clean and energy-efficient road transport vehicles.

(iii) society, as well as facilitation of the inventory analysis through a cost breakdown structure, among others. Consequently, this has been taken as a reference when defining the LCC approach to be followed in the CALIMERO project, along with additional peer-reviewed journal articles, specific economic documents and guidelines on LCC.

3.2 Methodological approach of life cycle costing

The following subsections have been divided in a consistent manner with that employed for the S-LCA proposed (see **Section 2.2**). This is due to the fact that, in the introduction of both ISOs which standardized the LCA method (i.e., ISO 14040 and ISO 14044), it is stated that although it is common practice for socio-economic aspects to be excluded from an LCA, these should be conducted in accordance with the methodological guidelines proposed in the environmental domain.

3.2.1 Goal and scope definition

As with LCA, the first step is to clearly define the objective of the assessment and the scope of the analysis. It is also important to define the target audience and geographical scope, as these choices can have a significant impact on the results, given that elements such as energy consumption, taxes and salaries are often linked to specific countries or regions.

The FU is also specified in this step, and it should be the same to the one defined in the LCA, based on physical properties or quality specifications, to ensure that the environmental and economic impacts can be combined (Valdivia et al., 2021). For multifunctional systems, a physical or economic allocation should be made. The defined system boundaries should also be consistent with the LCA and include all relevant stages based on the objective of the assessment.

Taking into account the work conducted by Bachmann et al. (2024) as a reference basis, this first step of the LCC should answer up to nine different topics in the form of guiding questions to settle an appropriate starting point. However, not all of them are related to the goal and scope definition, apart from there are some more in line with the description of further steps like inventory analysis or impact assessment. Then, the associated step(s) covered has/have been identified. The relative questions and answers have been summarized in **Table 16**.

Based on the information provided in **Table 16** of this report, it can be said that we worked out a cLCC (manufacturer perspective) and not an eLCC for several reasons:

- Solely, one specific environmental externality (i.e., external costs of environmental impacts caused by the company that are not included in the price) has been addressed, namely that related with GHG emissions (refer to **Section 3.2.3.6**) in the form of internal costs to be paid for producers. In addition, this is not presented separately for informative purposes to avoid double counting between LCA and LCC.
- Depending on the case study addressed, some of the life cycle stages have had to be neglected due to the availability of economic data information (e.g., EoL). In this sense, we have focused solely on a manufacturing company perspective, thus relegating the economic dimension of sustainability to the expenditures and profits associated with the evaluated product. The above was decided for facilitating both the task of economic evaluation when collecting the monetary information needed for the academic partners, apart from the economic interpretation when the results are transmitted to industrial partners. However, this simple inventory aggregation would be equivalent to considering only one impact category in the LCA. Then, to explore further in the state-of-the-art of this issue, some recent scientific publications were consulted about the economic evaluation beyond the profitability already addressed (see **Section 3.2.5**).

Table 18. Questions and answers for defining the goal and scope of the Life Cycle Costing methodology to be followed in the CALIMERO project.

#	Step(s) covered	Topic(s) addressed	Question	Answer
1	Goal and scope and inventory analysis	Audience and perspective	<i>From which perspective is the economic assessment intended to be undertaken?</i>	The economic assessment will be addressed in the context of the CALIMERO project, in which both academic and industrial partners will be involved. The former in LCC performance, while the latter in the data provision. Therefore, based on the origin of the primary information obtained, the selected perspective corresponds to the target audience: Manufacturing companies
2	Goal and scope and inventory analysis	Elements to be included in the assessment	<i>Will only costs be considered or also positive cash flows (e.g. revenues)?</i>	It will be considered both positive and negative cash flows
3	Goal and scope and inventory analysis		<i>Will only private effects be considered or also external effects? If so, in which way will they be monetized?</i>	External environmental effects will be considered by quantifying greenhouse gas emissions costs and setting a fixed price in terms of € per each ton of carbon dioxide equivalent emitted through the Emissions Trading System configured in a European Union context
4	Inventory analysis		<i>Can available, but confidential data be used?</i>	Considering the primary and private nature of the data used from the industrial case studies, this will not be available
5	Goal and scope and impact assessment	Temporal dimension	<i>Which time horizon is considered?</i>	As a mutual agreement, 10 years will be established as time frame
6	Goal and scope and impact assessment		<i>Is discounting of future cash flows (and also externalities) envisaged?</i>	Discounting effects for future cash flows will be considered within the time frame established by means of a common discount rate between all the CALIMERO case studies, while externalities (from CO ₂ emissions) remain outside of these effects
7	Goal and scope and inventory analysis	Spatial dimension and product system boundaries	<i>What is the spatial coverage (system boundaries) of the economic assessment?</i>	A cradle-to-grave approach will be proposed to be followed for the economic assessment, although some life cycle stages, such as EoL, are not relevant or hard to be included due to (partially) the consideration of a single stakeholder's perspective: Manufacturing companies
8	Goal and scope and inventory analysis		<i>Which life cycle stages are intended to be distinguished?</i>	All the case studies are relative to production processes of different bio-based industries, putting the focus on a single producer's perspective. Therefore, (raw) material extraction, manufacturing, distribution and maintenance will be covered, while some life cycle stages such as design and use, will be out of scope due to data availability constraints. Nevertheless, in the CALIMERO project is not the aim to distinguish between life cycle stages, but only to provide some economic information relative to a set of indicators selected
9	Goal and scope and inventory analysis		<i>Will capital goods (infrastructure and equipment) and overhead costs be considered?</i>	Capital goods are intended to be covered, although the kind of costs considered in each case study will vary depending on the availability of information

- According to an agreement between the CALIMERO project partners and in line with the most common way to proceed with this kind of economic assessments in the literature (Alejandrino et al., 2021), the following list of economic indicators is proposed to be estimated: Life Cycle Costing (LCC), Net Present Value (NPV), Levelized Cost of Production (LCOP), Internal Rate of Return (IRR) and Payback Period (PP). A more detailed description of each of them is collected in **Section 3.2.3**. However, due to the

product focus and the life cycle multi-stakeholder perspective of LCSA, the total undiscounted cost is recommended as the primary metric (Hunkeler et al., 2008), thus avoiding discounting to facilitate the alignment with LCA.

In general terms, it can be seen that there are several drawbacks when it is referred to opt for a cLCC in comparison with an eLCC when it comes to integration in an LCSA. This is despite the fact that the cLCC procedure selected complies with the main requirements settled in the CALIMERO project, which are based on the integration of a series of sustainability indicators into an MOO framework. It is for this reason that this issue will be one of the subjects for further discussion in WP5 (*Improvement of the Sustainability Performance of Bio-based Industries*) when elaborating a series of recommendations and guidelines to three key stakeholders: (i) industry, (ii) policy makers, and (iii) scientific community.

3.2.2 Inventory analysis

Once the main features and assumptions of the assessment have been defined, it is the turn of the economic inventory analysis, which should encompass those costs (and benefits) occurring throughout the life cycle of the products from the CALIMERO case studies to be analyzed. As it has been already mentioned, this inventory information must be referred to the same FU selected for the LCA (and S-LCA) to be aligned with the LCSA requirements. Moreover, all collected costs should be used the same currency. In this sense, due to the European context of the CALIMERO project, € has been selected.

Likewise, it is important to note that cost breakdown structure proposed by Bachmann et al. (2024) was not followed, since the differentiation of the economic impacts between life cycle stages is not one of their purposes. Therefore, the information to be collected for configuring the economic inventory appears below.

- OPEX (Operational Expenditures). Costs incurred to support an organization's day-to-day core operations, which can be direct (salaries, material costs, and energy/utilities) and indirect (e.g., rent or management).
- CAPEX (Capital Expenditures). Costs of acquiring, upgrading and maintaining physical assets such as property, plants, buildings, technology or equipment.
- Depreciation rate (optional). Percentage rate at which an asset is depreciated over its estimated productive life, as used in accounting to derive due tax payments.
- Maintenance rate. Cost required to maintain physical assets such as equipment or property. It is usually estimated on a percentage basis and depends on the CAPEX, but it might be adjusted based on the production capacity.
- Discount rate. Rate of return used to discount future cash flows to their present value. Future cash flows are discounted to reflect the time value of money. Because of inflation, interest rates, and opportunity costs, money is more valuable the sooner it's received.
- Inflation rate. The rate at which the general level of prices for goods and services is rising, and subsequently eroding the purchasing power of money. It is usually expressed as a percentage of the increase in the Consumer Price Index over a given period of time.
- Taxes. Contribution to state revenue on a percentage basis. Therefore, it will depend on the geographical and temporal situation of the study conducted.
- Sales. Relative to the life cycle stage "use", it corresponds to the gross profits from a

manufacturing company perspective.

- EoL costs (optional. Depending on manufacturer control of EoL, such as decommissioning, disposal or the valorization of residues (in this case, a revenue from selling the residue, notably machinery).

3.2.3 Impact assessment

A list of the indicators proposed for the economic assessment is provided below, along with an explanation of the environmental externality methodology used. The data requirements for each indicator are also summarized in **Table 17**.

Table 19. Economic indicators, level of assessment, description and data requirements.

Economic Indicator	Description	Data requirements
Life Cycle Cost (LCC)	Total expenditures during a life cycle	<ul style="list-style-type: none"> - OPEX: Operational expenditures <ul style="list-style-type: none"> ○ Yearly cost of materials ○ Yearly cost of energy ○ Yearly cost of water ○ Yearly cost of workers ○ Yearly cost of maintenance (if it is known, otherwise a 5% of CAPEX will be applied) ○ Yearly cost of EoL treatments (optional) - CAPEX: Capital expenditures like investments by means of: <ul style="list-style-type: none"> ○ Acquisition of physical assets ○ Upgrading of physical assets - Depreciation rate (optional): The default depreciation rate is 10%, but this can be adjusted depending on the life of the asset - Maintenance rate: It is usually calculated as the 5% of the CAPEX, but it might be adjusted based on the production capacity - Discount rate: A standard discount rate of 5% can be applied by default - Inflation rate: Usually expressed as a percentage of the increase in the Consumer Price Index of a region over a given period of time. - Taxes: Contribution to state revenue on a percentage basis. Therefore, it will depend on the geographical and temporal situation. - Time frame: Temporal extension in which the study is framed. It is usually considered by years (10 year for the CALIMERO case studies) - Level of production: In terms of FU in a given period of time (kg·year⁻¹, m³·year⁻¹, etc.). The same FU of the LCA or S-LCA it is recommended in order to ease conducting an LCSA - Sales: relative to the level of production in a given period of time (e.g., €·year⁻¹) - CO₂ emissions: An LCA can be conducted for estimating a carbon footprint in terms of CO₂ eq. emissions - CO₂ price: Tax to be paid relative to the CO₂ emissions
Net Present Value (NPV)	The sum of all the discounted future cash flows that considers the time value of money over the entire lifetime	
Levelized Cost of Production (LCOP)	Theoretical sales price to make the minimum average price ($C_0 = 0$) for a pre-defined lifespan. It can be used to evaluate the economic feasibility or to establish the sales price, since this should always be higher than LCOP to be cost-effective	
Internal Rate of Return (IRR)	Rate of return of the production system analyzed. The higher the IRR the better	
Payback Period (PP)	Time to recover the cost of an investment	
Environmental externalities (from CO ₂ emissions)	Price to be paid according to the CO ₂ emissions relative to a product system based on policy taxes	

3.2.3.1 Life cycle cost

The Life Cycle Cost (LCC) indicator measures all costs incurred during the life cycle stages of the

product system to be analyzed, for a reference period (**Equation 19**) (Bachmann et al., 2024).

$$LCC = \sum_{t=0}^T \frac{C_t}{(1+i)^t} \quad (\text{Equation 19})$$

Where:

- LCC: Life Cycle Cost (€)
- C_t: Total costs for time period t (e.g. for a producer perspective, this is CAPEX + OPEX + Maintenance + Taxes) (€)
- i: Discount rate (%), if applied total present/discouted costs. If zero, undiscounted costs
- t: Time year (year)
- T: Time frame (years)

3.2.3.2 Net present value

The Net Present Value (NPV) is the sum of all the discounted future cash flows (including costs and revenues) with the possibility of taking into account the time value of money over a time frame defined (**Equation 20**) (Rödger et al., 2018).

$$NPV = \sum_{t=0}^T \frac{N_t}{(1+i)^t} = \sum_{t=0}^T \frac{B_t - C_t}{(1+i)^t} \quad (\text{Equation 20})$$

Where:

- NPV: Net Present Value (€·year⁻¹)
- N_t: Net cash flow at time period t, calculated as cash inflow minus cash outflow (€·year⁻¹)
- B_t: Total positive cash flow for time period t, e.g., sales from a producer perspective (€·year⁻¹)
- C_t: Total negative cash flow for time period t, e.g., costs from a producer perspective. In this regard, the following aspects can be considered to be included: CAPEX, OPEX, maintenance and taxes (€·year⁻¹)
- i: Discount rate (%), if applied total present/discouted costs. If zero, undiscounted costs
- t: Time year (year)
- T: Time frame (years)

3.2.3.3 Levelized cost of production

The Levelized Cost of Production (LCOP) provides insights into the average cost per unit of product produced (**Equation 21**) (Reichelstein and Rohlfing-Bastian, 2015). LCOP indicates the minimum average price (C₀) at which the product must be sold to achieve the break-even point and cover production costs (i.e., when NPV is equal to 0). The lower the C₀, the more the product can be sold at a lower price, making it more competitive.

$$C_0 = NPV \cdot \left(\frac{i}{(1-(1+i)^{-T})} \right) \quad (\text{Equation 21})$$

Where:

- C₀: Cost of production/sales per unit of product produced to break even, i.e., earnings equal to zero (€·year⁻¹)
- NPV: Net Present Value (**Equation 20**) (€·year⁻¹)
- i: Discount rate (%)
- T: Time frame (years)

3.2.3.4 Internal rate of return

The Internal Rate of Return (IRR) represents the specific investment return of the production system, e.g., investment in capital to support production (Bianchi et al., 2020; Goedhart et al., 2015). The IRR is the discount rate at which the NPV equals zero, or in other words, the rate that equates the sum of the present value of expenses with the sum of the present value of anticipated revenues (**Equation 22**). The higher the IRR, the more desirable the investment is, as it will be more resilient to discounting effects.

$$IRR = (NPV = 0) \quad (\text{Equation 22})$$

$$IRR = \left(\sum_{t=0}^T \frac{N_t}{(1+i)^t} = 0 \right)$$

Where:

IRR: Internal Rate of Return (%)

NPV: Net Present Value (**Equation 20**) (€·year⁻¹)

N_t: Net cash flow at time period t, calculated as cash inflow minus cash outflow (€·year⁻¹)

i: Discount rate (%), if applied total present/discounted costs. If zero, undiscounted costs

t: Time year (year)

T: Time frame (years)

3.2.3.5 Payback period

The Payback Period (PP) represents the amount of time it takes to recover the cost of an investment. It is estimated through the ratio between the total investment and the average cash flows (revenue or savings) (**Equation 23**). However, considering the time dependence of the cash flows, the discounted PP can also be interesting to estimate, representing the period in which the cumulative NPV is equal to zero. In addition, the discounted PP has the peculiarity of focusing on both the profitability and the liquidity of the investments, as opposed to the NPV (profitability) and PP (liquidity), which consider only one of them (Bhandari, 2009).

$$PP = \frac{TI}{R} \quad (\text{Equation 23})$$

Where:

PP: Payback Period (year)

TI: Total investment (in a specific period of time) (€)

R: Average amount of revenues (or savings) per year over a time period (€·year⁻¹)

3.2.3.6 Environmental externalities

There are a variety of monetary valuation techniques that can be used to convert environmental impacts into economic terms. One of them is based on the assessment of damage costs for emissions and natural resource use, expressed in monetary terms using characterization and weighting factors. Consequently, this procedure is aligned with the LCA methodology by directly using the LCIs. On the downside, apart from the need to include several additional processes and their updating, it is important to note that these factors are expressed as global averages due to the often global scale of supply chains and global market trading of environmental damage costs, despite the lack of contextualization that this may also generate depending on the case study analyzed (Steen, 2019). Likewise, the monetary valuation method included in the Environmental Price Handbook is based on the prices associated with pollution (and other intangible forms of pollution such as noise), expressed in terms of social welfare losses (de Bruyn et al., 2023). However, the monetary valuation coefficients provided in this guide are tailored to the ReCiPe method, disregarding other LCIA methods such as the EF.

A recent literature review identified more than 50 suitable monetary valuation coefficients with the EF method, although with significant variability in the number of coefficients reported per impact category (e.g., 16 for climate change and 1 for water use). In addition, up to 6 different monetary valuation approaches (Amadei et al., 2021) were identified: (i) damage costs (costs that result from changes in natural capital), (ii) abatement costs (costs that mitigate, avoid, reduce, control, restore, or replace the damage), (iii) budget constraint (willingness to pay for an additional quality-adjusted life year, i.e., a life year lived with full well-being), (iv) averting behavior (cost of preventing or compensating for a change in the availability of a good), (v) market price (willingness to pay in an existing market for a good) and (vi) mixed approaches and other approaches (i.e., consideration of two (or more) or none of the above approaches). This situation highlights the need for a robust and common set of monetary valuation coefficients in line with the EF method.

Notwithstanding, the consideration of environmental externalities would imply double counting of the same impact (both from an environmental and economic point of view), which would lead to inconsistencies in future steps of the methodology to be implemented in the CALIMERO project. In this regard, when setting different objectives to be achieved within the MOO framework. For the analysis of the case studies covered by the CALIMERO project and with the purpose of avoiding double counting, we have only considered actual or foreseen financial costs related with environmental flows to be included in the (financial) LCC profile. In addition, when this indicator is considered, its accounting will be promoted externally to the LCC in order to know the monetary contribution of the environmental externalities to the total. Note that an alternative is to consider the monetization of externalities derived from LCA and S-LCA, with addition to eLCC results, as an expansion to LCSA where the total impact is then presented in monetary values. The optimization problem then would also only consider one monetary objective.

When it comes to actual or foreseen financial costs for environmental flows, the price for the GHG emissions (in terms of CO₂ eq.) have been considered, as they are financially traded in an EU context through the Emission Trading System (ETS). The ETS is a useful tool for controlling and making progress towards decarbonizing electricity producers and industrial companies in Europe in a cost-effective way. On the one hand, it requires industries to implement systems to monitor their emissions, and, on the other hand, it sets a maximum quota of allowable emissions that is reduced each year. However, it takes a business-friendly approach by making the total amount of emissions more flexible through its commoditization. This carbon market is regulated by fixed annual emission allowances that act as a currency. If a company does not want to pay the penalties for exceeding the set limits, it can buy allowances from other companies, while companies that do not exceed the limits can either keep them for another year or sell them to other companies for their own benefit. Thus, companies will see their emission reductions translated into economic incentives (European Commission, 2024).

Currently, the ETS covers about half of the EU's emissions, but it is being progressively updated to include emissions from shipping in 2024. Moreover, a new EU ETS was launched in 2023 and will be fully operational in 2027, called ETS2, covering emissions from fuel combustion in buildings, road transport and other small industries, which will lead to incentives for investments in building renovation and low-emission mobility. Therefore, the consideration of the ETS turns out to be interesting for the alignment of the CALIMERO case studies with the overarching EU climate goals of the European Green Deal (European Commission, 2019), apart from the European Climate Law (EU Commission, 2021).

Nevertheless, the ETS has experienced several price declines over the past decade due to the accumulation of allowances. To overcome this issue, a market stability reserve was created in 2019 to achieve a stabilization between the supply and demand of allowances. Since its introduction, the carbon price has increased from approximately €10 per ton of CO₂ eq. emitted in 2015 to €80 per ton of CO₂ eq. emitted in 2022. In the meantime, several price fluctuations have been produced under the context of an increasing tendency, although a stabilization of the price of about ±5€ is expected up to 2030 (varying between €70 and €75 per ton of CO₂ eq. emitted) thanks to the boost of decarbonization policies (Enerdata, 2023). Thus, in the case studies

where externalities are covered, it is proposed to quantify the GHG emissions costs as a fixed price of €75 per ton of CO₂eq. emitted in order to allow the comparability among the CALIMERO case studies analyzed. Likewise, this figure is in line to the average of several monetary valuation methods that take into account the abatement costs (i.e., those related to the mitigation, prevention, reduction, control, restoration or replacement of the damaged product) (Amadei et al., 2021; Entrena-Barbero et al., 2023).

3.2.4 Interpretation of results

In this final stage, the results of the LCI and/or LCIA are processed and reviewed to arrive at a final set of recommendations and conclusions from the assessment. The completeness of the study and the identification of limitations and uncertainties should also be analyzed and reported at this stage. Among the elements of the LCI, CAPEX and OPEX are considered particularly relevant to complement the selected economic indicators and will therefore be included in the interpretation phase.

3.2.5 Beyond economic profitability

The previous economic indicators selected to be evaluated have been focused solely on economic profitability in terms of expenditures and profits. However, this simple inventory aggregation would be equivalent to considering only one impact category in the LCA. Then, to explore further in the state-of-the-art of this issue, some recent scientific publications were consulted about the economic evaluation beyond the profitability already addressed.

Broadening the scope of the definition of economic sustainability, up to five additional aspects can be distinguished: (i) stability, (ii) autonomy, (iii) productivity, (iv) customers and (v) innovation (Arulnathan et al., 2022). Therefore, a number of additional indicators have been proposed. To do this, among other sources of information, a recent review conducted by Lago-Oliveira et al. (2024) about LCC indicators for monitoring the bioeconomy, has been taken into consideration. Nevertheless, it is important to note that these economic indicators have only been compiled as examples and that their subsequent application in the CALIMERO case studies is beyond the scope of the project.

3.2.5.1 Stability

Following a manufacturing company perspective, the best or worst economic stability organization can be determined by how well the identified risks are managed, as is presented in **Equation 24**. These risks can be described as bottlenecks in the form of investment episodes, government regulations, or constraints created by market dynamics (Yescombe and Farquharson, 2018). Moreover, one of the common strategies for managing risk is by including the level of diversification in terms of outputs, income streams, market access, apart from the technologies used. An example of this is shown in **Equation 25**. However, it is crucial to keep in mind that the economic stability of a company is not guaranteed by its diversification, since it also depends on several additional factors, such as the structure of the diversification itself, the size of the company, the characteristics of the sector under study, among others (Neugebauer et al., 2016).

Another factor that can be representative of a company's stability is its success, which is influenced, among other aspects, by the level of satisfaction that its employees have. To estimate the above, an average employee satisfaction rate on several different topics can be measured in specific metrics such as in a 5-level ratio: e.g., very satisfied (2), satisfied (1), neutral attitude (0), dissatisfied (-1) or very dissatisfied (-2) (see **Equation 26**). In this way, qualitative information is transformed into quantitative data. To do this, primary information should be prioritized by conducting surveys. However, employee satisfaction can also be understood in a negative way, for example, by considering the number of complaints in a given period. On the other hand, this indicator is influenced both directly and indirectly by a number of drivers: the level of employee loyalty, job satisfaction, management communication, employee engagement, employee retention and

employee rewards, thus creating synergies with other economic dimensions of sustainability (e.g., productivity and customers) (Al Kurdi et al., 2020).

$$\text{Management of risk aspects} = \frac{\text{number of risks identified}}{\text{number of risks managed}} \quad (\text{Equation 24})$$

$$\text{Diversification} = \frac{\text{number of products}}{\text{number of markets}} \quad (\text{Equation 25})$$

$$\text{Employee satisfaction } (-2, -1, 0, 1, 2) = \sum \text{level of satisfaction of specific topics} \quad (\text{Equation 26})$$

3.2.5.2 Autonomy

Autonomy reflects the ability to which an economic system is physically self-sufficient, i.e., in terms of the resources or goods it requires. Moreover, self-sufficiency is not only referred to in physical terms, but also according to the monetary flows. Indeed, the latter can be associated with a relatively novel concept that is being included in the evaluation of sustainability when assessing a product system, namely, criticality. This is a specific feature that materials can have if they have a high economic importance and simultaneously entail a risk when it comes to guaranteeing their supply, thus translating into higher production costs (Graedel and Reck, 2016).

The relative contribution of third-party financing from stock issuance, bonds issuance or bank loans (see **Equation 27**) entails a reflection of the greater or lesser degree of autonomy a company may have (Fakhroni et al., 2022). The same applies to the level of reliance, which can be calculated through the percentage of imports, both at the mass or monetary level, relative to the total inputs needed, as is shown in **Equation 28** (Wood and Hertwich, 2013). Similarly, in addition to import dependency, the contribution to exports can also be considered when comparing the firm with the rest of the industry in a given geographical context or when estimating the level of revenue involved.

The amount of public economic benefits received in the form of subsidies will also play a fundamental role in the level of autonomy of a company. However, it should also bear in mind that, although beneficial in economic terms, they can be counterproductive in a holistic perspective of sustainability, as they can lead to environmental detriments (Kletzan-Slamanig et al., 2023)

$$\text{External financing } (\%) = \frac{\text{income from third-parties}}{\text{total net income}} \cdot 100 \quad (\text{Equation 27})$$

$$\text{Reliance on imports } (\%) = \frac{\text{imports}}{\text{total inputs}} \cdot 100 \quad (\text{Equation 28})$$

3.2.5.3 Productivity

When productivity is referred to, it is measured by considering the amount of output produced relative to a given input. Similarly, the productivity of a firm or production process is usually estimated per labor or capital.

With regard to labor productivity, this economic indicator is usually related at the country level, since it reflects the level of quality of life in a social context, in the sense that it represents a higher amount of goods and services consumed (at an increasingly reasonable price) in the same amount of working time. From the above, it can be deduced that this dimension of economic sustainability is related to many others due to its relationship with physical and human capital, apart from investment in new technologies. It is then that this indicator is commonly estimated by applying the Gross Domestic Product as the economic output related to the total amount of hours worked. However, in the case of contextualization to the micro level (i.e., economic evaluation of specific production systems), this can be changed for the Gross Value Added (GVA) (Thomassen

et al., 2009), understood as the relative economic contribution of a company in a region (see **Equation 29**).

Moreover, capital productivity is a way of showing the potential of capital used to produce output in the form of income, thus reflecting the overall efficiency of production. Then, the net income obtained is divided by the average value of the total capital, as shown in **Equation 30**. Capital can refer to several types, such as human, natural, or social capital, but in LCC literature it is commonly referred to as fixed capital (e.g., infrastructure, machinery, etc.) (OECD, 2015).

$$\text{Labor productivity } (\text{€} \cdot \text{h}^{-1}) = \frac{\text{gross value added } (\text{€})}{\text{hours worked } (\text{h})} \text{ (Equation 29)}$$

$$\text{Capital productivity} = \frac{\text{net income } (\text{€})}{\text{average value of total assets } (\text{€})} \text{ (Equation 30)}$$

Finally, it is important to take into account the external socio-environmental context when assessing both labor and capital productivity, which have been shown to be threatened by global warming due to climate change. In this sense, several studies link the increasingly frequent episodes of extreme temperatures or heat waves (environmental consequences) to episodes of cognitive and learning unproductivity (socio-economic consequences) (Lai et al., 2023). Moreover, both indicators need to be measured over a period of time or compared to similar firms to support their interpretations.

3.2.5.4 Customers

Customers in the sense of their interests or consumption preferences can be integrated into the LCC as an economic aspect following two different perspectives. On the one hand, from an economic point of view in, by means of official statistics that represent the market share (**Equation 31**). This is a relatively easy and direct way to measure it, and although it usually be estimated through secondary information, it helps to understand the importance that a certain product may have within its sector for a given social context (Neugebauer et al., 2016). On the other hand, from a social point of view, customer satisfaction can be rated by considering the maximum willingness-to-pay (in monetary terms) of a specific product, minus its internal production cost (see **Equation 32**). To estimate this, primary information should be prioritized by carrying out surveys. Nevertheless, customer satisfaction can be also understood from a negative side, considering the number of complaints related to the product in a certain period of time (Lago-Oliveira et al., 2024).

$$\text{Market share } (\%) = \frac{\text{total sales of a specific product } (\text{€})}{\text{sales of the product evaluated } (\text{€})} \cdot 100 \text{ (Equation 31)}$$

$$\text{Customer satisfaction } (\text{€}) = \max(\text{willingness to pay} - \text{internal production cost}) \text{ (Equation 32)}$$

3.2.5.5 Innovation

This is a factor of paramount importance in ensuring the sustainability of a company over time. In this sense, an improvement in innovation can lead to the release of a new product in the market (stability in terms of diversification), the granting of external financing that contribute to the autonomy of the firm, and the increase in labor productivity or customer satisfaction, which would be translated into a better productivity and customer performance. Therefore, from the above it is clear that innovation can influence the rest of the economic impact categories (Gault et al., 2023).

This concept includes up to six factors: (i) innovation culture, (ii) strategy, (iii) knowledge and competence, (iv) organizational structure, (v) research and development activities and input, and (vi) financial innovation performance. Due to its multifaceted nature, it is both difficult and abstract to translate innovation into a simple indicator. In fact, it can be measured both qualitatively and quantitatively, and several methods for its estimation are currently available in the literature. However, some examples are provided in relation to

the following aspects of innovation: knowledge and competence (**Equation 33**), research and development activities and input (**Equation 34**), and financial innovation performance (**Equation 35**) (Dziallas and Blind, 2019):

Innovation = number of managers trained in the methods and tools of innovation (**Equation 33**)

Innovation (%) = share of research budget from a total company budget (**Equation 34**)

Innovation (€) = new – to – (market/business) sales (**Equation 35**)

4 CONCLUSIONS AND FUTURE PROSPECTS

This report examines the social and economic assessment methodologies which follow a life cycle approach. Thorough research was carried out to define the S-LCA (Social Life Cycle Assessment) and LCC (Life Cycle Costing) scope and methodological framework to be implemented in the CALIMERO case studies, taking into account some specificities of the bio-based industry. With this in mind, a set of social and economic indicators was selected to be included in the LCSA (Life Cycle Sustainability Assessment) of the 5-target bio-based industries of the CALIMERO project. The selected set of life cycle indicators was mainly justified by their ability to be integrated into the MOO (Multi-Objective Optimization) framework to be developed, taking into account the previous expertise of the partners. Therefore, it represents a set that could potentially be used to assess certain key aspects of social and economic performance of bio-based systems, although further efforts should be made to develop and implement a more comprehensive list of quantitative indicators covering other social and economic facets and stakeholders. Nevertheless, the two calculator tools provided with this report (based on the JCP (Job Creation Potential) assessment and a list of economic indicators) can pave the way for their rapid replication, adaptation and further refinement by stakeholders focused on developing LCC and S-LCA methodologies.

Regarding S-LCA, in the case of the JCP, it was recognized that the inclusion of job losses due to bio-based activities is important to obtain a complete and more accurate picture of the employment situation. However, it was found that methods based on assumptions or outdated approaches are widely used in the literature, increasing the uncertainty of the results. In view of these challenges, higher data accuracy has been a priority in this report and therefore only job creation has been used to assess employment through the JCP indicator, building largely further on the framework of Pillain et al. (2019). Nevertheless, it is important that future research focuses on developing a more complete methodology that accurately captures both job creation and job losses. In expansion of the JCP calculation, a more accurate level of the type of jobs created was achieved in terms of worker skills and gender.

In relation to the assessment of some aspects related to OHS (Occupational Health and Safety), “indoor health impacts” was explored in terms of occupational exposure to hazardous chemicals and translated into an S-LCA indicator targeted to the “worker” stakeholder group. The idea of this indicator is to highlight the systematic work environment management related to identification, risk assessment and compliance with the regulated OELs (Occupational Exposure Limits) for relevant substances. Using this indicator could provide insights into the occupational hygiene measures in the workplace, which include actual exposures (e.g., wood dust, emissions of terpenes, particles and diesel exhaust from work vehicles, etc.) that are not necessarily captured in the assessment based on raw materials and chemicals in the production process. By adopting several different approaches to evaluate work environment risks, one can better get an overall picture and thus better assess performance and responsibility within the area of OHS.

Also, in the context of OHS, in this report a series of missing toxicity CFs (Characterization Factors) have been predicted through ML (Machine Learning) approaches within the USEtox and EF (Environmental Footprint) frameworks, focusing on emissions into household and industrial indoor air. Given the complexity of chemical toxicity data, apart from the high cost and regulatory limitations of experimental testing, this approach

offers a solution to estimate CFs only based on chemical descriptors derived from SMILES (Simplified Molecular Input Line Entry System) representations. However, the pipeline used clustering with GMM (Gaussian Mixture Models) to ensure chemicals were grouped based on molecular similarity, enhancing the understanding of prediction accuracy. From the two models used (i.e., XGBoost and Gaussian process), the overall alignment of both suggests that they are capturing similar patterns, being XGBoost more accurate, thus suggesting that the Gaussian process has a slightly lower but comparable predictive capacity, although it is important to bear in mind that this latter model provided confidence intervals, which may add value in assessing predictive uncertainty, a key consideration in toxicity risk assessments. Besides, for some clusters, Gaussian process outperforms XGBoost, which is helpful to select the better model to predict chemicals CF in those clusters. The general findings obtained highlight the potential of ML to extend CF coverage for life cycle impact assessment in the absence of comprehensive experimental data, supporting OHS and environmental management. Notwithstanding, further refinements, including expanded descriptor sets and other ML algorithms, may improve model performance and generalization across diverse chemical classes.

As an additional option for characterizing occupational risks relating to chemical exposure, we have calculated CFs for the method ProScale. The method is relatively simple to apply, but there is anyway an issue to assess substances if they lack hazard statements in REACH (Registration, Evaluation, Authorization and Restriction of Chemicals Regulation). There we have tested a set of hazard prediction tools that have been developed in other contexts. The work indicates that it is possible to expand the list of substances possible to assess with this approach by applying computational prediction methods, based on QSAR and other types of read-across-based approaches. Further distinction of substances missing hazard classification to substances being considered safe, and substances simply having data gaps, is needed in the continued work. Please note, that the characterization factors as presented in this report, need further scrutiny before they can be applied in any specific LCA study. This is, specific exposure and environmental compartment conditions need to be considered.

With respect to the economic dimension, the LCC indicators selected are focused exclusively on the monetary profitability of bio-based manufacturing companies. Yet, it is of paramount importance to consider that the monetary benefits of a particular company may not be aligned with a benefit to society (e.g., workers or local communities) or nature (e.g., in terms of increased biodiversity). The above is related with the fact that our economic assessment has been configured from a producer perspective, lagging behind other key stakeholders such as consumers or society (Bachmann et al., 2024). To pave the way towards a more holistic approach, the focus on economic sustainability has been expanded, by including stability, autonomy, productivity, customers and innovation aspects (Arulnathan et al., 2022). Up to twelve indicators were proposed in this regard. Consequently, these indicators should be taken as a first approach to broaden the focus when it is referred to the inclusion of the economic dimension in the LCSA, since these additional aspects could potentially be considered as mid-point impact categories, although until arrive this point, it is important to deal with three main aspects: (i) the alignment of the indicators with a life cycle perspective (for instance, on a recurrent basis these can lead to difficulties when the LCA (Life Cycle Assessment) practitioner has to represent the indicator in relation to the selected FU, (ii) avoid any overlapping that may exist when addressing socio-economic aspects (the clearest example of this would be the economic analysis of customers through the LCC and the social analysis of consumers through the S-LCA), (iii) broadening the scope to other stakeholders beyond manufacturing companies.

Likewise, environmental externalities were proposed to be analyzed in order to estimate the damage to nature caused by the economic impacts. In this concern, the diversity of monetary valuation coefficients, especially in relation to the EF method, highlights the critical need for a standardized set of coefficients to maintain consistency across environmental assessments and impact methods. Consequently, future efforts should aim at defining these coefficients according to the environmental impact assessment methods used. In addition, a great deal of information has been identified in the equations of the economic indicators that is difficult to extract by industrial partners and that, in many cases, assumptions have to be made based on

previous studies in the literature, implying an important focus on the uncertainty of the results obtained, so that more efforts should be made in this aspect with the aim of obtaining reliable primary data. In our approach, we have solely considered the financial costs from the GHG emissions estimated through an LCA in terms of CO₂ eq. related with the ETS system due to its current or near-future uptake. In the context of the ETS, many emission sources have recently been included in this system to make it as representative as possible and to make it a reference at the European level. However, there are additional emission sources associated with bio-based production and consumption systems, such as those from biogenic sources, that have not yet been included.

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