



Linking inventories and impact assessment models for addressing biodiversity impacts: mapping rules and challenges

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Abstract

Purpose An adequate matching between the nomenclature of elementary flows in life cycle inventory (LCI) databases and life cycle impact assessment (LCIA) methods is key for ensuring the proper application of life cycle assessment (LCA). However, the nomenclature of elementary flows lacks harmonization among the LCA community. This paper aims at defining mapping rules and discussing main challenges related to the process of systematically mapping LCI nomenclatures to LCIA methods and models addressing biodiversity impacts.

Methods Eight LCIA methods and models addressing biodiversity loss are analyzed: five comprehensive LCIA methods (i.e., LC-IMPACT, Impact World+, Ecological Scarcity 2013, ReCiPe 2016, and Stepwise), one land use intensity-specific LCIA model; and two approaches adapting the GLOBIO model to LCIA. These models and methods are mapped to two LCI nomenclatures (ecoinvent v3.6 as implemented in Simapro and Environmental Footprint (EF) 3.0). A mapping tool was developed to support the process of (a) mapping elementary flows by name, Chemical Abstract Service number or available synonyms; (b) implementing specific mapping rules regarding compartment/sub-compartment, and substance name; (c) mapping elementary flows to manually defined proxies (e.g., synonyms, spelling corrections and similar substances); and (d) assigning characterization factors (CFs). The process entails analyzing a case study to identify uncharacterized elementary flows.

Results and discussion We present a mapping of LCIA methods and models addressing impacts on biodiversity loss with specific LCI nomenclatures. Mapping rules are proposed for elementary flows regarding chemicals, carbon emissions, land use, water use, and particulate matter. Specific aspects to be considered in mapping elementary flows in LCIA and LCI nomenclatures are discussed. Main gaps in LCI nomenclatures are associated to toxicity and climate change impacts. The EF 3.0 was more aligned than ecoinvent 3.6 with the LCIA methods and models regarding elementary flows coverage and regionalization level. Analyzing uncharacterized flows revealed further coverage needs for “Chemical, organic” (between 19 and 20% uncharacterized flows), “Chemical, inorganic” (between 9 and 18% uncharacterized flows) and “Chemical, radioactive” (between 9 and 14% uncharacterized flows).

Conclusions This paper contributes to the operationalization of LCIA methods and models addressing biodiversity impacts by proposing a systematic mapping process and rules for a better LCIA-LCI connection. Different development pathways of LCI (e.g., focused on substance name detail) and LCIA (e.g., towards improved regionalization level) have stretched the gap between both nomenclatures. Recommendations are provided identifying further efforts towards the harmonization of the nomenclature of elementary flows in the LCA community.

Keywords Nomenclature · LCI-LCIA connection · Impact assessment · Interoperability · Life cycle assessment · Life cycle inventory

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1 Introduction

Life cycle assessment (LCA) is a systematic quantitative method to assess the environmental impacts of products, which supports decision-making and policymaking (Sala

et al. 2021). At the EU level, the European Commission has developed the Product- and Organisation- Environmental Footprint (PEF and OEF, respectively) methods to ensure comparable results when comparing products in the EU market (EC 2013, 2021). Several life cycle inventory (LCI) databases, life cycle impact assessment (LCIA) methods, and LCA software have been developed so far, enabling an improved operationalization of LCA as a method for environmental impact assessment of products and processes. Although some nomenclature harmonization efforts have taken place in the LCA community (see e.g., EC-JRC 2010; Koellner et al. 2013a), most parallel developments have not been harmonized, leading to several inconsistencies and a lack of interoperability. This has been accelerated by the rapid development of both LCI and LCIA, which has led to a multiplication of elementary flows, use of different substance names (Edelen et al. 2018), and different uses of compartments and approaches to regionalization. Such lack of interoperability may impair the robustness of LCA results (Lopes Silva et al. 2019; Herrmann and Moltesen 2015), the combined use of different LCI databases (Ingwersen 2015; Suh et al. 2016), and the use of common elementary flows among LCA data (Edelen et al. 2018).

As mentioned above, the parallel development of LCI databases and LCIA methods has resulted in a mismatch among nomenclatures (Edelen et al. 2018). This challenges the classification and characterization of LCI during the LCIA step, which may result in a number of uncharacterized flows when conducting LCA studies (see e.g., Castellani et al. 2017) that might be not accurately assessed by practitioners, adding uncertainty to the results. These mismatches are difficult to be handled by LCA practitioners, since the mapping of the flows requires specific knowledge of the considered LCIA impact pathways, namely the pressures underpinning the impacts (e.g., which type of impacts are caused by a specific substance), impact models, and the rules followed in the classification stage of the LCIA step. These mapping challenges are well reflected in the implementation of LCIA methods in, e.g., the ecoinvent database (Hischier et al. 2010).

The limited operability of LCIA methods due to the mismatch with LCI databases generally prevents the direct implementation of LCIA developments by LCA practitioners, as it requires a previous detailed mapping, or may lead to an improper mapping compromising the robustness of the results. This is particularly relevant in decision-making, as different results due to unmapped flows might hamper the robustness of LCA results being at stake (Lopes Silva et al. 2019; Herrmann and Moltesen 2015). In the context of LCIA developments, refining the modelling of environmental impacts or addressing emerging environmental concerns, as well as enabling the mapping between LCI databases and new LCIA methods, is crucial for their mainstream use and operationalization, as well as for being widely applied on case studies by LCA practitioners. For example, the assessment of biodiversity loss at the

endpoint level is still under refinement in the LCIA community. A number of LCIA methods have been developed over time and are available under different levels of operationalization (i.e., from provision of CFs to LCIA methods implemented in LCA software) (Crenna et al. 2020). Limitations in connecting LCIA methods and LCI databases are currently hampering the widespread use of more sophisticated and robust impact assessment methods and models.

International and multi-stakeholder efforts have recently focused on these issues within the United Nations Environment Programme (UNEP)'s Life Cycle Initiative (GLAD 2021). To address data interoperability and access, the Global LCA Data Access (GLAD) network was launched in June 2020 to allow users to access and convert datasets from different providers (UNEP 2021). On the other hand, the Global Guidance on Environmental Life Cycle Impact Assessment Indicators (GLAM) project aims at recommending a global LCIA method for selected impact categories. For overcoming barriers in the connection between LCI-LCIA, a specific subtask has been established to enhance the interoperability effort of the reference nomenclature and data format, and to identify and harmonize the most relevant elementary flows, and handle group emissions (i.e., elementary flows representing a group of substances such as 'pesticides, unspecified') (UNEP, 2020). Within the GLAM framework, a study performed through a multi-stakeholder group reviewed the key issues and gaps related to the LCI-LCIA connection (UNEP 2020). Four groups of issues were identified: (a) inconsistencies in nomenclature, correspondence and data format between LCI and LCIA; (b) specification and level of details; (c) modelling limitations (i.e., clear boundaries between LCI and LCIA); and (d) data quality requirements. An analysis of inconsistencies highlighted the lack of interoperability of nomenclature for LCI-LCIA among key stakeholders (developers of LCI databases, LCIA methods and LCA software).

This paper aims at defining mapping rules and discussing the main challenges in the process of systematically mapping LCIA methods and models assessing endpoint impacts on biodiversity to LCI nomenclatures. The analysis focuses on biodiversity loss (damage on ecosystems quality). In this regard, a mapping process is defined and applied to the selected methods, which was implemented through a self-developed mapping tool. Furthermore, a case study is assessed with the mapped methods to analyze and spot uncharacterized elementary flows.

2 Methods

This section presents the selected LCIA methods and models, and LCI nomenclatures, and describes the systematic mapping process followed to maximize the connection between LCIA and LCI nomenclatures.

2.1 LCIA methods and models

This analysis focuses on LCIA methods and models addressing biodiversity loss, with different underpinning approaches (Crenna et al. 2020): LCIA methods, a land use-specific LCIA model and the GLOBIO model, which is a biodiversity impact assessment model developed beyond LCA and is potentially applicable. The assessment of biodiversity loss is performed at the endpoint, considering the damage to the area of protection (AoP) ecosystem quality (Woods et al. 2018). The selection was based on the following criteria (Table 1): representation of midpoint and/or endpoint impact assessment methods, different levels of coverage of impact categories (i.e., from single impact categories to comprehensive methods), levels of operationalization (ranging from requiring self-derivation of CFs to methods implemented in commercial software), and levels of regionalization (from only global default factors to highly regionalized methods). The study thus includes five global LCIA methods (Ecological Scarcity 2013, IMPACT World+, LC-IMPACT, ReCiPe 2016, Stepwise 2006), a land use-specific LCIA model (land use intensity-specific CFs) (Chaudhary and Brooks

2018), and two LCIA approaches based on the GLOBIO model (Schipper et al. 2016). A brief description of each of the selected methods and models is provided below. An in-depth analysis of the selected LCIA methods and models is provided in the supplementary materials (Table SM1.1).

Ecological scarcity 2013 The Ecological Scarcity 2013 (from here onwards refer to as Ecological Scarcity) is a “distance-to-target” method (Frischknecht and Büsler 2013). Ecological Scarcity is a method that characterizes the impacts in eco-points (or UBP’s, *Umweltbelastungspunkte*), a unit to characterize and weight the 11 different impact categories and allowing for their aggregation into a single value by means of a distance to target approach based on Swiss environmental targets. Among the 11 impact categories, only the land use addresses damage to ecosystem quality (biodiversity loss).

Impact World+ Impact World+ is a globally regionalized method for LCIA, which is resulting from the evolution of IMPACT 2002+, LUCAS, and EDIP methods (Bulle et al. 2019). Impact World+ presents both midpoint and endpoint

Table 1 Overview of the LCIA methods selected in this study in relation to the selection criteria

	Ecological Scarcity 2013	Impact World+	LC-IMPACT	ReCiPe 2016	Stepwise 2006	Chaudhary	GLOBIO v 3.5
Type	LCIA method	LCIA method	LCIA method	LCIA method	LCIA method	Land-use specific LCIA model	Biodiversity assessment model
Midpoint impacts		x		x	x		
Endpoint impacts	x	x	x	x	x	x	x
Impact categories	11	18	11	17	15	2	2
Categories addressing biodiversity	1	13	7	9	7	2	2
Implemented in LCA software	SimaPro, Gabi, OpenLCA	No	No	OpenLCA	No	No	No
Available CSV file for SimaPro implementation		SimaPro (midpoint and damage version, global and continental version)	No (provision of CFs)	SimaPro (midpoint, endpoint)	SimaPro	No (provision of CFs)	No (derivation of CFs)
Regionalization level	Country (for water flows)	Global, continental, biomes, watershed and finer resolutions (the finest 0.5°×0.5°)	Global, continental, country, ecoregions, watersheds, river basins and finer resolutions (the finest 0.05°×0.05°)	Global, continental, country	Global	Country, ecoregion	Global

impact indicators: 18 midpoint impact categories, from which 13 contribute to the AoP ecosystem quality (biodiversity loss, in PDF·m²·y) at the endpoint level. The level of regionalization (native scale) depends on the impact category: terrestrial and freshwater acidification (resolution of 2° × 2.5° (latitude × longitude)), freshwater eutrophication (resolution 0.5° × 0.5°), ecotoxicity (continental), water scarcity (sub-watershed), and land transformation/occupation (biome). The resolution scale of the method includes four levels: global default, continental, country, and native.

LC-IMPACT The LC-IMPACT method provides only endpoint CFs for 11 impact categories, 7 of them being related to ecosystem quality (biodiversity loss, in PDF·y) (Verones et al. 2020). As for Impact World+, the level of regionalization in LC-IMPACT depends on the impact category. Impact categories contributing to biodiversity impacts include spatial differentiation: photochemical ozone formation (world regions), toxicity (subcontinental regions), acidification (resolution 2° × 2.5°), freshwater and marine eutrophication (freshwater ecoregions and river basins to large marine ecosystems), land stress (terrestrial ecoregions), and water stress (resolution 0.05° × 0.05°). In addition to CFs at the native scales, LC-IMPACT also provides country, continental, and global averages.

ReCiPe 2016 ReCiPe 2016 (from here onwards refer to as ReCiPe) is an update of ReCiPe 2008 (Goedkoop et al. 2013; Huijbregts et al. 2016), providing both midpoint and endpoint indicators. Covering a total of 17 midpoint impact categories, the endpoint assessment of the AoP ecosystem quality (biodiversity loss, in species·y) is covered by 9 impact categories. ReCiPe provides global generic CFs but also provides country-level CFs for four categories contributing to biodiversity impacts: photochemical ozone formation, terrestrial acidification, freshwater eutrophication, and water use.

Stepwise 2006 The Stepwise 2006 method (from here onwards refer to as Stepwise) combines characterization models from IMPACT2002 + v. 2.1 and EDIP2003 methods (Weidema 2008). Indicators are provided both at the midpoint (15 impact categories) and endpoint levels, with 7 indicators contributing to the AoP ecosystem quality (biodiversity loss, in Biodiversity Adjusted Hectare Years (BAHYs)). CFs in Stepwise are not regionalized, so only global default factors are available.

Land use-specific model Chaudhary and Brooks (2018) recently developed a LCIA model focusing on land use intensity-specific (LUIS) CFs in order to calculate global biodiversity impacts of products. This model is based on the countryside species-area relationship (SAR), which

is parametrized based on three land management intensity levels to calculate the endpoint impact on biodiversity loss (in PDF·y). CFs are provided at country scale and terrestrial ecoregion levels. Global generic CFs were obtained from one of the authors (personal communication with Abhishek Chaudhary). Despite addressing a single impact category (land use), this model has been selected as it is the further development of the model selected (as interim recommendation) for addressing biodiversity impacts due to land use in GLAM (UNEP 2016), i.e., Chaudhary et al. (2015).

GLOBIO GLOBIO is a global biodiversity model developed by the PBL (Netherlands Environmental Assessment Agency), UNEP GRID (Global Resource Information Database)-Arendal and UNEP-WCMC (World Conservation Monitoring Centre) (Schipper et al. 2016). It links different drivers of biodiversity loss (climate change, land use, infrastructure, and nitrogen deposition) to impacts on biodiversity in terms of mean species abundance (MSA). GLOBIO integrates the IMAGE modelling framework to analyze global changes driven by human activities in the long term. To explore the adaptation of the GLOBIO model to the context of process-based LCA, two main approaches are investigated to derive LCIA-based CFs, namely the biodiversity footprint (BF) (Hanafiah et al. 2012; van Rooij and Arets 2016; Wilting et al. 2017; Wilting and van Oorschot 2017) and the global biodiversity score (GBS) (CDC Biodiversité 2019). Both BF and GBS are based on GLOBIO version 3.5, the one adopted in this study by means of the generation of two sets of CFs: GLOBIO-BF (in MSA loss·m²·y) and GLOBIO-GBS (in MSA loss·m²). CF derivation is performed for climate change and land use drivers addressing impacts to terrestrial species (Table 2). Regarding climate change, the factor $4.37 \cdot 10^{-1} \text{ MSA loss} \cdot \text{m}^2 \cdot \text{yr} \cdot (\text{kg CO}_2)^{-1}$ for a 100-years' time horizon (Wilting et al. 2017) and the global warming potential for each substance $(\text{kg CO}_2 \text{eq} \cdot (\text{kg substance})^{-1})$ (IPCC 2013) are employed. Concerning impacts due to land use, MSA values for each land-use type from the GLOBIO model are employed (Schipper et al. 2016).

2.2 LCI nomenclatures

These LCIA methods and models were mapped to two different LCI nomenclatures. A mapping is proposed to the widely used ecoinvent 3.6 (Wernet et al. 2016). This database was chosen as a LCI nomenclature for which implementation exercises of LCIA methods and corresponding mapping rules already exist (Hischier et al. 2010). This nomenclature was used as implemented in SimaPro 9.1 (Pré Consultants 2020), from which the list of elementary flows was extracted. SimaPro software was selected due to the availability of at least one LCIA method (i.e., Ecological

Table 2 CF derivation formula and impact unit for the adaptation of the GLOBIO v3.5 model to LCIA, by impact category and approach

Approach	Impact category	CF derivation formula	Impact unit
Biodiversity footprint (BF)	Climate change	$4.37 \cdot 10^{-1} \left(\frac{MSA_{loss-m^2 \cdot y}}{kgCO_2eq.} \right) \times GWP \left(\frac{kgCO_2eq.}{kg_{substance}} \right)$	MSA loss-m ² ·y
	Land occupation	MSA loss ^a	MSA loss-m ² ·y
	Land transformation	$MSA_{loss} \times \frac{RP^b}{2}$	MSA loss-m ² ·y
Global biodiversity score (GBS)	Climate change	$\frac{4.37 \cdot 10^{-1}}{100y} \left(\frac{MSA_{loss-m^2 \cdot y}}{kgCO_2eq.} \right) \times GWP \left(\frac{kgCO_2eq.}{kg_{substance}} \right)$	MSA loss-m ²
	Land transformation	MSA loss ^a	MSA loss-m ²

^aMSA loss equals 1-MSA, where MSA values are retrieved from GLOBIO v3.5 (Schipper et al. 2016), ^bRP, restoration period, assumed as 20 years (Brandão and Milà i Canals 2013)

Scarcity) at the time this exercise started (November 2019), the provision of CSV files for SimaPro implementation by some LCIA method developers (Table 1), and the availability of a case study covering a wide range of consumer goods (Sala and Sanyé Mengual 2022; Sala and Castellani 2019; Sala et al. 2019), which easily allows assessing the uncharacterized flows (see Sect.2.3.4), being this a specific feature of the software.

For comparative purposes, the LCIA methods and models were also mapped to the Environmental Footprint (EF) 3.0 nomenclature (as per the reference package released in 2018 (EC-JRC 2018)).

2.3 Mapping process between LCI and LCIA nomenclatures

Implementing an LCIA method means a proper classification and an adequate matching of the two nomenclatures (namely LCIA and LCI). This enables the correct quantification of the potential environmental impact caused by each environmental pressure (i.e., elementary flows representing emissions to the environment and resource use). Elementary flows are composed of three elements: substance name (i.e., name of material, energy, or space); compartment and sub-compartment) (i.e., flow context); and flow unit. They can also include additional information, such as the CAS@

number or synonyms (Edelen et al. 2018). All these elements are key in ensuring a successful LCI-LCIA connection and were addressed in this study.

When mapping LCI nomenclatures to LCIA methods and models, four situations can occur (Fig. 1):

- A direct match is found between the elementary flow in the LCI nomenclature and the LCIA method, resulting in a mapped flow with a CF (Situation 1)
- No direct match is found between an elementary flow in the LCI nomenclature and a CF in the LCIA method due to the following:
 - Differences in LCIA and LCI nomenclatures (Situation 2)
 - No CF is available in the LCIA method for an elementary flow present in the LCI nomenclature, assuming this elementary flow was expected to be classified to the specific impact category (Situation 3)
 - No elementary flow exists in the LCI nomenclature to match the provided CF in the LCIA method (Situation 4)

Considering these situations, a systematic mapping process was defined to maximize the LCI-LCIA connection to improve the operationalization of the available biodiversity

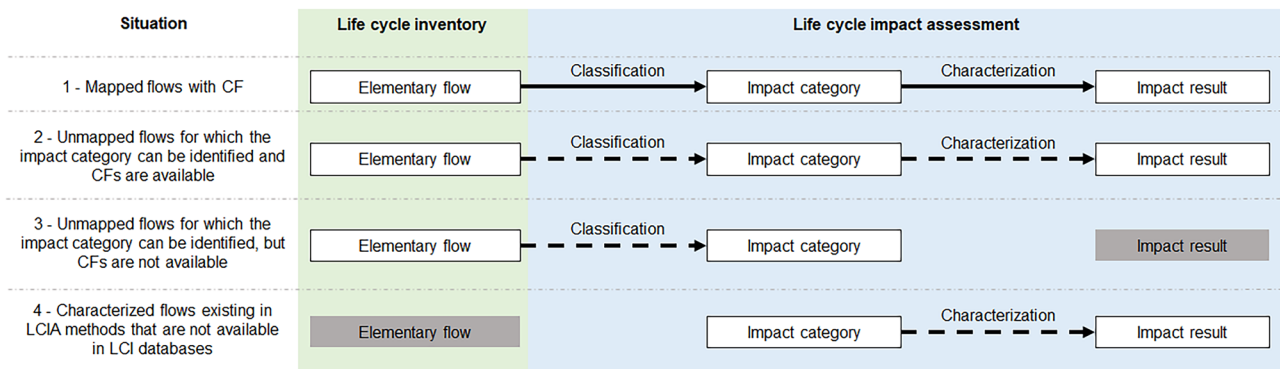


Fig. 1 Possible situations when mapping LCI databases and LCIA methods. LCI-LCIA connection depends on existing elements (white boxes) and missing elements (gray boxes), which can lead to an established connection (solid line) or an absent connection (dashed lines)

impact assessment models. The different steps and decision tree of the mapping process are detailed in Fig. 2 and described below. The mapping of LCIA methods was supported by a Java mapping tool developed in this study and representing a common practice in interoperability studies to minimize the occurrence of errors (e.g., Suh et al. 2016). The mapping tool required three main inputs: (i) the LCIA methods in the original nomenclature system including CFs (source flow list); (ii) the LCI nomenclature (target flow list); and (iii) the mapping rules to match the context and

substance name of both nomenclatures (context mapping file). The information is provided to the mapping tool in a machine-readable format. Concerning the EF 3.0 nomenclature, Step 4 (implementation to a case study) was excluded. The mapping of the CFs derived from models addressing specific categories (LUIS, GLOBIO) was performed manually due to the relatively low number of elementary flows involved (i.e., Steps 2 and 3). The mapping process resulted in files (in CSV format) to be imported into SimaPro for ecoinvent 3.6 and in ILCD-compliant data packages (in XML

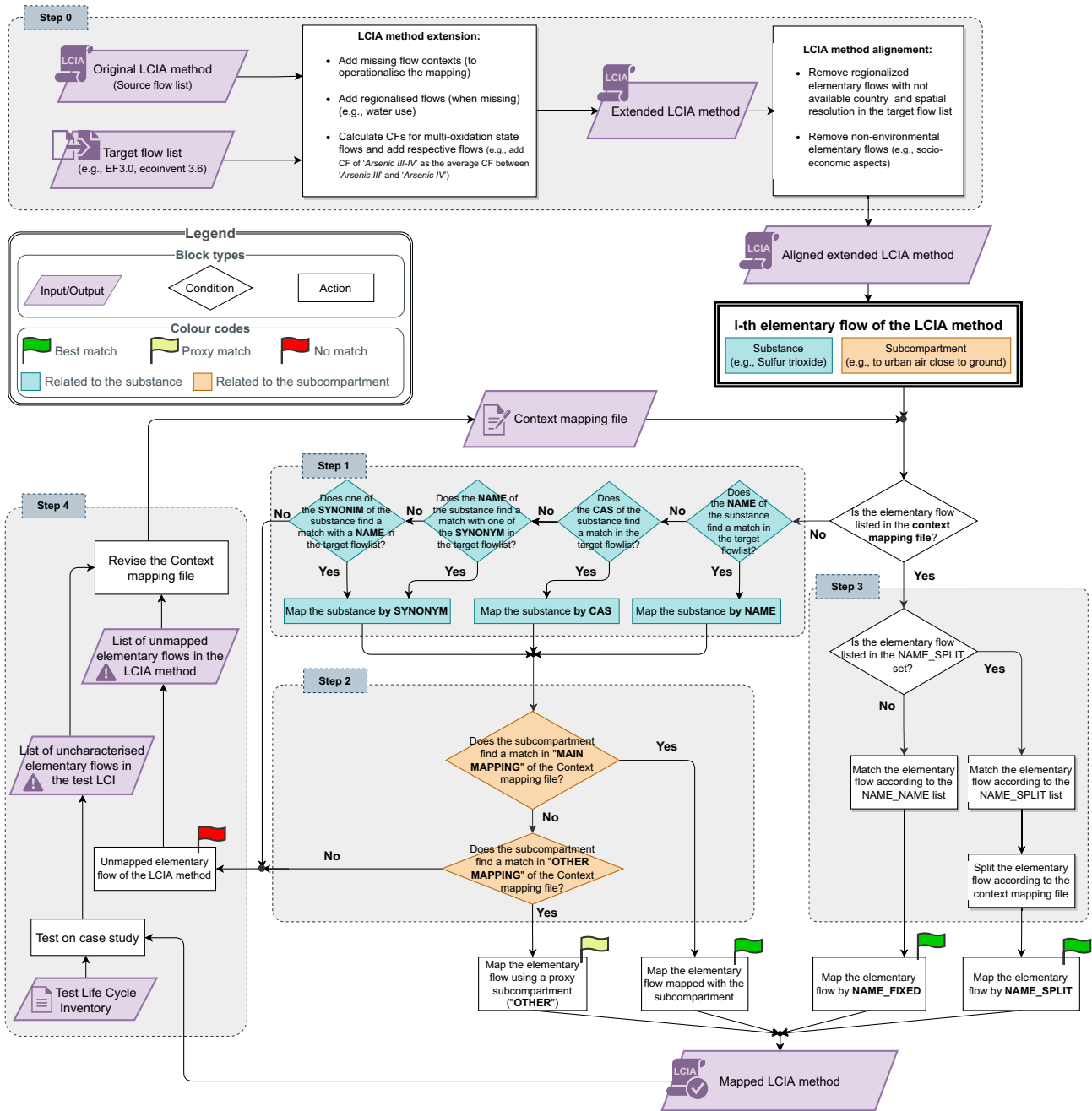


Fig. 2 Mapping process and decision tree (including input/outputs, actions and decisions) followed in this study, by step

format) to be used in the Look@LCI software (Zampori et al. 2018) concerning the EF 3.0 nomenclature.

2.3.1 Step 0: alignment between flow list of original LCIA method with target flow list

As a preparatory step for the mapping process, the list of elementary flows of the original LCIA methods was aligned with the target flow list (LCI) originating two versions of the LCIA method:

- First, the methods were extended to add missing flow contexts (this helped to operationalize the mapping, as a subcompartment is required to define an elementary flow), add regionalized flows when missing (e.g., water use flows), and add elementary flows for those substances with multi-oxidation states (for which a CF was also calculated). This resulted in the “extended method.”
- Then, some elementary flows were discarded for the mapping process to align LCIA methods with the scope and level of regionalization of the LCI nomenclature (e.g., aspects not covered in the LCI nomenclature like socio-economic aspects). This resulted in the “aligned extended methods,” which are the starting point for the mapping procedure.

2.3.2 Step 1: automated mapping

A first step (only for LCIA methods) included the automated mapping of elementary flows with the same substance CAS® or name in both LCI and LCIA, or with corresponding synonyms, where available. This step followed a hierarchical order, as detailed in the decision tree (Fig. 2): CAS®, substance name, and synonym. Such automated identification between nomenclatures corresponds to situation 1 (Fig. 1). This step simulates the automatic mapping that the SimaPro software would perform when importing the provided CSV files, potentially leading to unmapped flows due to mismatch in the nomenclature (Situation 2, Fig. 1) or the undesired addition of new elementary flows not present in the LCI (Situation 4, Fig. 1). These two situations were prevented in the mapping process by mapping exclusively those elementary flows present in the LCI nomenclature (target flow list) through the alignment process in Step 0.

2.3.3 Step 2: manual context mapping

The provision of context in an elementary flow is essential to determine directionality (i.e., being a LCI input or output) and properly implement an LCIA method (Edelen et al. 2018). Since the context of elementary flows was not harmonized among LCI and LCIA nomenclatures, a manual

mapping of compartments and subcompartments was necessary. Some compartment-subcompartment pairs in the LCI nomenclature were available in the LCIA methods, while for the remaining ones, an allocation to the unspecified compartment or a proxy was performed. The context mapping was also structured hierarchically by proximity rules: the best possible match between compartment-subcompartments in the source (LCIA nomenclature) and the target (LCI nomenclature) was defined, which were collected as “main mapping” for the context. Additional proxies were provided in the case that the flow was not available in the specific context in the target nomenclature, as “other mapping.” For example, for an “emission to air urban close to ground” flow in the source nomenclature (LCIA), the hierarchy in the target nomenclature (LCI) can be, in order, “emission to air urban close to ground,” “emission to air low stack,” and “emission to air unspecified.” In the case the context of the substance was unavailable in all the proxies defined, it was labelled as unmapped.

2.3.4 Step 3: manual substance mapping

Apart from correspondence tables between the LCIA method (source list) and the LCI (target list) for subcompartments and possible proxy subcompartments, the context mapping file also includes flow-specific mapping resulting from a manual check of the unmapped flows (particularly of substance name). For the LCIA models (i.e., LUIS and CFs derived from the GLOBIO model) all elementary flows were mapped manually, while for the five LCIA methods, this step was applied only for those flows not mapped automatically in Step 1. The manual mapping yielded both one-to-one (NAME_NAME list) and one-to-many (NAME_SPLIT list) correspondence tables that are fine-tuned in an iterative approach. Elementary flows mapped according to the one-to-one correspondence are labelled as “NAME_FIXED,” while elementary flows mapped by the one-to-many list are labelled as “NAME_SPLIT” (Fig. 2). Note that the mapping tool developed for this study iteratively excluded flows to be mapped automatically by capturing ex-ante manually mapped flows, as detailed in the decision tree (Fig. 2). Despite of being a time-consuming effort, this was necessary to prevent unmatched flows due to differences in nomenclature between LCI and LCIA. In those cases where the LCIA method was implemented in SimaPro (i.e., Ecological scarcity) or a CSV was already available, this step also reviewed the proposed mapping by the LCIA method developers. This step focused on (a) identifying aleatory mismatches due to, e.g., syntax errors, synonyms, and CAS® numbers repetition for regionalized flows; (b) systematically mapping certain groups of flows (i.e.,

chemicals, carbon, land use, water, particulate matter); and (c) defining mapping rules for other issues identified in uncharacterized flows from Step 4 (e.g., level of detail in substance name).

2.3.5 Step 4: case study

In order to identify possible gaps and recurrent problems in the matching between the elementary flows present in the LCI database and the LCIA methods, the mapped methods were tested in a case study. This was done for the five LCIA methods and the LCI nomenclature as implemented in SimaPro and available in the case study (ecoinvent 3.6). Due to the limited number of covered impact categories and of elementary flows, the LCIA models (i.e., LUIS and the two sets of CFs derived from the GLOBIO model) were excluded from this step and not implemented to the case study. The employed case study was the Consumption Footprint, a process-based LCI model aiming to assess the environmental impacts of EU consumption with a full bottom-up perspective by modelling the life cycle of around 140 representative products of five areas of consumption: food, mobility, housing, appliances, and household goods (Sala and Castellani 2019; Sala et al. 2019). This case study was selected due to the large representativeness of processes and associated environmental impacts leading to a wide coverage of elementary flows in the LCI. The comprehensive list of elementary flows is available in Supplementary Material (Table SM1.2).

The uncharacterized elementary flows from the case study were evaluated to identify mapping gaps and improve the existing mapping. This iterative process allowed improving the mapping with the inclusion of new matches or the addition of proxies in Step 3. To systematically check for potential matches and detect recurrent issues, all uncharacterized elementary flows were grouped into 14 major groups according to the nature of the elementary flows (including the differentiation between resources and emissions):

- Chemical inorganic
- Chemical inorganic, groups
- Chemical metal
- Chemical metal, groups
- Chemical organic
- Chemical organic, groups
- Chemical other
- Chemical other, groups
- Chemical other, particulates < 10 μm
- Chemical other, particulates > 10 μm
- Chemical radioactive
- Chemical radioactive, groups
- Land use
- Water use

Two additional groups were created but excluded from Step 4, a priori: waste, because being mainly technical flows, these are usually not characterized; and raw material, since these flows contribute to the AoP on resources rather than to AoP on ecosystem quality. The employed categorization of elementary flows differed from the one provided by Edelen et al. (2018) due to two main aspects: the categories referring to chemicals were further disaggregated to represent different chemical typologies (i.e., organic, inorganic, metal) and the classification of chemicals was refined regarding specific potential impacts (i.e., particulates, radioactive).

3 Results

This section presents the mapping rules defined, the analysis of the resulting mapped LCIA methods and models, and the classification of the uncharacterized elementary flows resulting from the case study.

3.1 Definition of mapping rules

The definition of mapping rules was elaborated for the context of elementary flows and the substance name for different groups of elementary flows.

3.1.1 Context mapping

The context of the elementary flows (i.e., compartment and subcompartment) of the five LCIA methods evaluated in this study was manually mapped to the context categories in the ecoinvent nomenclature (Table SM1.3). Most of the missing compartment-subcompartment pairs were mapped to the unspecified subcompartment of the given compartment (e.g., air/(unspecified)), in alignment with the implementation of LCIA methods in ecoinvent (Hischier et al. 2010). Specific proxies were assigned to long-term emissions and for emission to “air, stratosphere” in Impact World+ after discussion with the LCIA method developers.

A source of mismatching between the elementary flows of the LCI databases and the LCIA methods was the lack of CFs for “unspecified” subcompartments in the LCIA methods, which can result in an LCI elementary flow being uncharacterized (e.g., an emission to “water, unspecified” is not characterized when the CF provided in the method is only for emissions to “water, ocean”). To solve such gaps, CFs for the “unspecified” subcompartment were added when required by considering the CFs of other subcompartments. The rules applied depended on the compartment (Table 3): precautionary principle for soil emissions (highest CF), average CF of high- and low-population subcompartments for air, and dependence on the impact category for water (i.e., river CF for terrestrial and freshwater-related impact

Table 3 Rules for identifying the CF for additional unspecified-subcompartment flows

Compartment	“Unspecified” subcompartment CF assignment rule
Soil	The highest CFs among the available sub-compartment are assigned to the “unspecified” following a precautionary principle
Air	Average between CFs of high pop and low pop sub-compartments
Water	The CFs of the “river” sub-compartment are assigned to “unspecified” for terrestrial and freshwater impact categories The CFs of the “ocean” sub-compartment are assigned to “unspecified” for marine impact categories

categories, and ocean CF for marine impact categories). These rules were adapted from the ecoinvent implementation (Hischier et al. 2010), following a discussion with LCIA method developers.

3.1.2 Chemical flows

Two main aspects were addressed in mapping chemicals: the nomenclature of the substance name and the oxidation states of metals. Chemical nomenclatures represented a challenge due to the different nomenclature strategies adopted in LCI and LCIA. Chemicals can be identified using IUPAC names (e.g., “1-Butanol”), common names (e.g., “Acetaldehyde”), commercial names (e.g., roundup), or other specific nomenclature systems (e.g., CFC-10). However, LCI and LCIA nomenclatures combined all these options rather than using a specific one creating a variety of synonyms that hampered the identification of individual chemicals among different nomenclatures and arose the complexity of correctly matching flows to guarantee high-quality results. Within LCIA methods, this heterogeneity partially depended on the impact assessment model used to characterize each impact category. For example, methods relying on USEtox® adopted its nomenclature (e.g., LC-IMPACT). As a result, chemical flows were carefully matched by reviewing all available synonyms for a given substance.

Mismatches in the metals with different oxidation states were found not only in the nomenclature of the substance name but also in the CAS® number. Mapping rules for metals were thus proposed considering both substance name and CAS® number (Table SM1.4). Main issues arose from the reporting of metals with no oxidation state or only including the cationic form in the LCIA methods. Two criteria were used to solve such mismatching situation for toxicity-related impact categories. Both criteria were deemed reasonable as already applied in the development of toxicity-related impact categories of the EF 3.0 method (Saouter et al. 2020), agreed with USEtox® (Rosenbaum et al. 2008) developers, and in

alignment with ecoinvent implementation (Hischier et al. 2010).

First, in case that only one oxidation state was present (e.g., Cadmium II) in the LCIA method, the same CF of the metal with a specific oxidation state was attributed to the uncharacterized metal with no specified oxidation state (e.g., Cadmium). This was implemented in the LCIA method by creating additional elementary flows equal to the ones pertaining to the metal with a specific oxidation state and changing the fields of the substance name and CAS® number to the metal with no oxidation state.

Second, in case that two oxidation states were reported, the CF of the uncharacterized metal was calculated as the arithmetic mean of the CFs of metals with oxidation state. This situation occurred for antimony (Sb III and Sb V), arsenic (As III and As V), and iron (Fe II and Fe III). For chromium, despite two states were available (Cr III and Cr VI) in the LCIA, only the CFs of Cr VI were here applied, being not only the most toxic but also the most bioavailable form in the environment. Alternatively, a precautionary approach could have been considered for all metals.

3.1.3 Carbon flows

Specific mapping rules were defined for carbon dioxide, carbon monoxide, and methane flows in relation to the emission origin (fossil, biogenic, and land transformation) (Table SM1.5). While the LCI nomenclature also included substances with unspecified origin, these were not always present in the LCIA method. In these cases, “fossil” origin was selected for carbon dioxide and carbon monoxide as a proxy. Conversely, “Methane, unspecified” was mapped with “Methane, biogenic” due to the relevance of biogenic sources in methane emissions (Kirschke et al. 2013). This is particularly relevant for case studies analyzing food products considering the meaningful role of methane emissions in food production processes, e.g., livestock or rice paddles. Missing carbon flows addressing land transformation as the origin of the emission (e.g., “Carbon dioxide, land transformation”) were mapped to the respective carbon flow representing a biogenic source in alignment with the PEF method (EC-JRC 2021). However, the latter choice opposes the indications for carbon dioxide in the ecoinvent implementation (Hischier et al. 2010).

3.1.4 Land use flows

In the case of land use flows, two main issues hampered an automatic LCI-LCIA connection. The first was related with differences in nomenclature between LCI databases and LCIA methods, which were aligned to the LCI nomenclature (e.g., in LC-IMPACT, Occupation/Transformation, to/

from pasture was changed to Occupation/Transformation, to/from pasture and meadow) (Table SM1.6). Such differences result from the fact that no harmonized implementation of the naming of land use flows and their detail level has been performed in the different LCIA methods and models, despite the proposed harmonized nomenclature by Koellner and colleagues (2013a). This proposed nomenclature was adopted in ecoinvent 3.0 and has been revised in subsequent releases (e.g., the land use class “arable” has been changed to “annual crop” in most recent versions).

The second issue concerned the level of detail for land use flows which was much higher in LCI nomenclatures. On the one hand, four levels of detail can be used in ecoinvent (including general land use (“agriculture”), land use specification (“arable”), land management (“non-irrigated”), and land use intensity (“extensive”)) (in alignment with Koellner et al. 2013a). Missing land use flows representing higher level of detail were mapped to the corresponding class in less-detailed levels (e.g., “Occupation, permanent crop, vine” was characterized with CFs from “Occupation, permanent crop”) (Table SM1.6).

On the other hand, some general land use categories (level 1 of Koellner’s classification) were missing in LCIA methods. In these cases, mapping rules were defined for five types of land occupation flows based on practices in other LCIA methods, relevance of the flows in terms of environmental impact, and presence in LCI case studies.

- Natural land uses: those land covers defined as natural references in Koellner et al. (2013a, b) were not mapped with a proxy unless a CF was already provided in the method. These natural land uses include forest, natural; grassland, natural (non-use); unspecified, natural (non-use); wetland, coastal (non-use); wetland, inland (non-use); sea and ocean; shrub land, sclerophyllous; snow and ice (non-use); and bare area. Note that some of these natural land uses have not yet been addressed in LCA, such as seawater bodies since most of the LCIA methods focus on terrestrial habitats (e.g., LC-IMPACT, IW +, and ReCiPe).
- Unknown or unspecified land use flows: the highest CF was mapped to these flows when no indications were provided in the LCIA method, following a precautionary principle.
- Artificial freshwater bodies: LC-IMPACT, IW +, and ReCiPe use different versions of SAR models (de Baan et al. 2013; Chaudhary et al. 2015) to calculate the CFs for land occupation. However, no method considered “water” to be a land use type, resulting in unmapped water occupation flows. To map these flows, we considered that both methods use the local land occupation CFs (CF_{loc}) to calculate the land use impact. CF_{loc} measures the relative decrease in species richness between a spe-

cific land use type and a (natural) reference habitat (varying between 0 and 1), where the higher the CF_{loc} , the higher the impact per land use type. Since the occupation of terrestrial ecosystems with water bodies gets a CF_{loc} of 1 (the highest possible) (Dorber et al. 2020), we applied a precautionary principle and used the highest available land occupation CF as a proxy for the land occupation regarding artificial freshwater bodies (i.e., water bodies, artificial; water courses, artificial; lakes, artificial; and inland waterbody, unspecified).

- Seabed bodies: Flows regarding seabed bodies were unmapped, as most of the LCIA methods focus on terrestrial habitats (e.g., LC-IMPACT, IW +, and ReCiPe). Although land use impacts on seabed bodies are still not available in the analyzed LCIA methods, there is some knowledge of impacts on this type of land use (Woods and Verones 2019).
- Snow and ice: Flows regarding occupation with artificial snow and ice were unmapped, as LCIA methods and models did not provide CFs for this specific land use category. Since there is a lack of CF_{loc} values for snow and ice occupation (Chaudhary et al. 2015), the magnitude of the impact remains unknown and we decided not to use any proxy CF for this type of land use.

Finally, land use transformation flows required adjustments to align LCIA methods to the way land transformation is handled in ecoinvent (i.e., including both directions “transformation to” and “transformation from” flows). In LCI, land transformation refers to a change in the ecosystem quality and distinguishes the transformation from the previous use (transformation from) to the current one (transformation to). Instead, land occupation flows indicate a delay in the recovery to the natural reference state (Milà i Canals et al. 2007). In ecoinvent, LCIs usually include both directions of land transformation (from and to); “transformation from” flows compensate for a portion of the impact of the “transformation to” flows (which are calculated as the integral of the difference in ecosystem quality between the land use situation and the reference situation over the regeneration time (Koellner et al. 2013b)) by taking into account the different levels of ecosystem quality between the previous land use and the reference situation (e.g., a transformation from arable land to artificial land potentially impacts to a lower extent biodiversity compared to a transformation from natural forest to artificial land). For example, the dataset “building construction, budget hotel, BR” includes the flows “Transformation, from urban, continuously built” and “Transformation, to urban, continuously built,” both with the same value (684.44 m^2) resulting into no impacts due to land transformation. Towards aligning with this land transformation approach in ecoinvent, both LC-IMPACT and LUIS were adjusted by adding the required transformation flows

Table 4 Presence and sign of CFs of land transformation flows in the methods covering land transformation, and implemented adjustment during the mapping process

Method	Transformation from		Transformation to		Mapping adjustments
	Present in method	Sign	Present in method	Sign	
IW	Yes	-	Yes	+	
LC	No		Yes	+	Inclusion of “transformation from” flows with the same CF value but with a changed sign of the corresponding “transformation to” flow
RCP	Yes	+	Yes	-	
GLO-BF	Yes	-	Yes	+	
GLO-GBS	Yes	-	Yes	+	
LUIS	No		Yes	+	Inclusion of “transformation from” flows with the same CF value but with a changed sign of the corresponding “transformation to” flow

to properly measure the impact in alignment with ecoinvent implementation (Hischier et al. 2010) (Table 4). Note that ReCiPe employed a different approach, where only natural land transformation is included, resulting in negative CFs for “transformation from” and positive CFs for “transformation to.” This aspect needs to be considered when interpreting LCIA results.

3.1.5 Water flows

Water use elementary flows (raw materials compartment) among the LCIA methods were not including all the water flows available in the ecoinvent nomenclature and proxy rules were defined (Table SM1.7). Ocean or saltwater flows were not mapped with proxies unless these subcompartments were available in the original methods (e.g., Impact World+). This rule considered that LCIA methods usually focus on impacts due to freshwater use (e.g., ReCiPe and LC-IMPACT).

In the case of LC-IMPACT, two specific aspects were also addressed. Firstly, “water, well, in ground” was only mapped for the extended version of the method. Secondly, “water, turbine use” should not be mapped as it represents an “in-situ” water use, while this method only quantifies impacts of consumptive water use (Verones et al. 2020). Although this is in line with other of the LCIA methods considered (e.g., ReCiPe), LC-IMPACT required specific attention due to the lack of a provided CSV file by method developers already considering ecoinvent modelling approaches. Therefore, as in the case of land use flows, alignment to the way water flows are modelled in ecoinvent was required. For example, the dataset “Electricity, high voltage {AT}, electricity production, hydropower, pumped storage” includes an input flow of “water, turbine use, unspecified natural origin” (1.183 m³), which is mostly returned to nature in the output flow “Water, AT” (1.15817 m³). Since input and

output flows employ a different substance name, not characterizing “water, turbine use” can lead to reduced or negative results. To prevent misleading results, “water, turbine use” was also mapped for LC-IMPACT with the corresponding CF of water flows (i.e., only one water flow is provided in the method).

3.1.6 Particulate matter flows

No harmonization was found in the nomenclature of substances addressing the emissions of particulate matter to air. In this case, the role of the subcompartment was a key as some nomenclatures (e.g., Impact World+) included the subcompartment in the substance name. This led to some level of redundancy, which has been already identified as an obstacle for interoperability in LCA nomenclatures (Edelen et al. 2018). The proposed mapping for these flows considered the substance name, paying specific attention to the particle size and the subcompartment, which are the drivers of the resulting impact (Table SM1.8).

3.1.7 Other mapping issues

A number of uncharacterized flows occurred due to different reasons than the ones explored above. The manual mapping of substance name included an evaluation of synonyms, different word patterns in the substance name composition, and syntax errors.

Synonyms are usually less used than CAS® as clarifying information associated to an elementary flow (Edelen et al. 2018). Synonyms were systematically checked to identify new mapping pairs between LCI and LCIA. This was of particular relevance for the use of nomenclatures (both LCI and LCIA) originating from different world regions (e.g., British vs. American English).

Different nomenclatures can use different word patterns hampering an automatic matching between them. For example, the origin of a resource can be specified together with the resource name (resource, origin) or including additional information (resource, specification, and name). As well, the redundancy of information in elementary flows can occur when compartment-subcompartment information is also included in the substance name (Edelen et al. 2018). Different patterns and redundancies were evaluated in the manual mapping step (e.g., particulate matter in Impact World+).

Syntax errors in flow naming (e.g., extra or missing characters, capitalization, and spaces) may hinder the mapping between LCI and LCIA nomenclatures (Edelen et al. 2018). The syntax of substance names was aligned to the ecoinvent nomenclature, including the following: (a) capitalization, (b) abbreviations, (c) conjunctions (e.g., and vs. &), (e) corrected misspelling and errors (e.g., shrubland vs. scrubland, grassland), (f) punctuation (e.g., commas, points, parenthesis), (g) use of plural and singular forms (e.g., deserts, mangroves, artificial water bodies), and (h) truncation (e.g., SimaPro accepts substance names with 40 characters, so longer descriptions of the elementary flows are truncated).

3.2 Mapping for LCIA methods and models addressing endpoint impacts on biodiversity

The LCIA methods and models were mapped to the ecoinvent nomenclature as implemented in SimaPro (Supplementary material 2). Table 5 summarizes the mapping process in terms of number of flows, from the original method to the resulting mapped method. The number of elementary flows refers to the unique combination of compartment, subcompartment, and substance and regionalization (when specified). In this regard, it is important to remark that in the native ecoinvent 3.6 nomenclature system, regionalization of elementary flows is addressed at the model level. In contrast, in the flow list of ecoinvent as implemented in SimaPro, the regionalization is specified in the substance name at the elementary flow level. The adaptation of the original methods and the level of coverage of the resulting mapped methods are further evaluated in this section.

With regards to the mapping process, the manual mapping of substance name was the most relevant step for two of the LCIA methods and for all the LCIA models (which were fully mapped manually) (Fig. 3). On the contrary, the use of CAS® numbers to identify substances (mainly chemicals) largely supported the automatic mapping (> 55%) for three of the LCIA methods. This highlights the relevance of using unique identification numbers in substances in mapping exercises, which could enhance the implementation of automated mapping procedures.

3.2.1 Adaptation of original methods

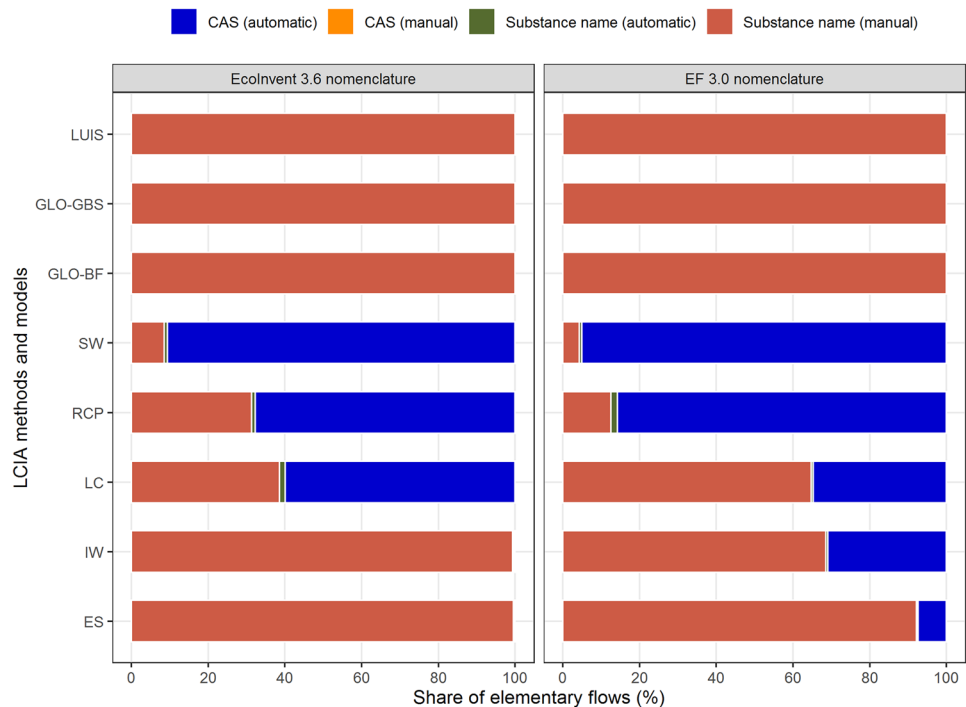
LC-IMPACT and Impact World+ were the methods with the largest number of elementary flows in the original versions (Table 5), being the ones with the largest presence of regionalized flows (Table SM4.1). On the contrary, LCIA models covering a limited number of impact categories included less than 260 flows in the original versions, apart from LUIS with a higher spatial resolution (more than 7000 flows) (Fig. 4a). The original methods required an adaptation to be mapped to the LCI nomenclature that included an extension with additional flows and an alignment to the scope and level of regionalization.

Additional elementary flows were added to the original LCIA methods and models to be aligned with the LCI nomenclature in terms of flows and context. The “extended methods” increased the number of flows of the methods between less than 0.4% (Ecological Scarcity, Impact World+, ReCiPe, Stepwise) and 340% (LUIS) (Table 5, Fig. 4a). This difference was mainly related to the operationalization level of the original methods, where those methods already implemented in SimaPro or with available CSVs for SimaPro implementation required the addition of fewer flows. Additional flows in the “extended methods” were associated to four main aspects: level of detail of substances, alignment with LCI modelling approaches, oxidation state of metals, and level of detail of flow context. Firstly, a different level of detail between LCIA and LCI nomenclatures required the use of the same CF of the LCIA method for several elementary flows of the LCI nomenclature. This occurs for land use flows where LCIA methods usually provided a limited number of CFs associated to general land use categories (e.g., annual crops) while LCI nomenclatures employed further levels of detail (e.g., annual crops, irrigated) (Table SM1.6). Other examples of this addition of elementary flows are water flows (e.g., in LC-IMPACT these were generic) (Table SM1.7) or carbon flows (e.g., where the origin of the emission can be indicated in the substance name) (Table SM1.5). Secondly, land use flows and water flows required the addition of new elementary flows to be aligned to the LCI modelling of land transformation (see Sect. 3.1.4) and turbine water use (see Sect. 3.1.5), respectively. Thirdly, new elementary flows were created in the case of metals for those cases of two oxidation states present in the LCIA method against an undefined metal in the LCI nomenclature (i.e., without specification on the oxidation state) (see Sect. 3.1.2). For example, the average of CFs associated to “Arsenic III” and “Arsenic IV” emissions to air-indoor was associated to the additional flow “Arsenic III-IV” created in LC-IMPACT to be mapped to “Arsenic” in the LCI nomenclature. Finally, elementary flows were created to align with the level of

Table 5 Number of flows in original, extended, aligned extended and mapped methods, by LCIA method and LCI nomenclature. Uncharacterized flows of the case study are presented for the mapping withecoinvent 3.6. The assessment includes Ecological Scarcity 2013 (ES), Impact World+(IW), LC-IMPACT (LC), ReCIpe 2016 (RCP), Stepwise (SW), GLOBIO-BF (GLO-BF), GLOBIO-GBS (GLO-GBS) and land use intensity-specific model (LUIIS)

LCI nomenclature	Descriptors	LCIA methods and models									
		ES	IW	LC	RCP	SW	GLO-BF	GLO-GBS	LUIIS		
Mapping withecoinvent	Original method (n flows)	2529	90,247	142,421	54,516	9685	256	242	7380		
	Extended method (n flows)	2539	90,297	209,111	54,530	9710	351	305	25,338		
	Aligned extended method (n flows)	1740	47,478	114,523	49,985	9701	351	305	103		
	Final mapped method (n flows)	1194	6488	15,326	6230	2217	171	129	103		
	Coverage (%)										
	Mapped/extended	47.0	7.2	7.3	11.4	22.8	48.7	42.3	100.0		
Mapping with Environmental Footprint	Mapped/aligned extended	68.6	13.7	13.4	12.5	22.9	48.7	42.3	100.0		
	Case study uncharacterized (n flows)	1780	1384	1381	1444	2259	-	-	-		
	Extended method (n flows)	4099	130,815	385,211	56,124	9876	1666	1606	39,637		
	Aligned extended method (n flows)	4041	130,194	305,441	56,124	9867	1666	1606	39,637		
	Final mapped method (n flows)	3703	121,942	303,765	54,473	9646	1658	1600	36,024		
	Coverage (%)										
Mapped/extended	90.3	93.2	78.9	97.1	97.6	99.5	99.6	90.9			
Mapped/aligned extended	91.6	93.7	99.5	97.1	97.7	99.5	99.6	90.9			

Fig. 3 Share of elementary flows in the mapped methods to ecoinvent LCI nomenclature, by mapping step. The assessment includes Ecological Scarcity 2013 (ES), Impact World+ (IW), LC-IMPACT (LC), ReCiPe 2016 (RCP), Stepwise (SW), GLOBIO-BF, GLOBIO-GBS, and land use intensity-specific model (LUIS)



detail of the context (compartment-subcompartment) of the LCI nomenclature. In particular, the “unspecified” compartment was added when missing in the original methods, such as in LC-IMPACT.

Once methods were extended, some elementary flows were discarded for the mapping process to align LCIA methods with the scope and level of regionalization of the LCI nomenclature. The “aligned extended methods” resulted in the reduction of between around 0.1% (Stepwise) and 47.4% (Impact World+) of the elementary flows of the “extended method” (Table 5), apart from LUIS with the highest level of reduction (99.6%) (Fig. 4a). On the one hand, the elementary flows discarded were associated to aspects not covered in the LCI nomenclature, such as noise flows in Ecological Scarcity or injuries in Stepwise. This issue affected a very limited number of flows. On the other hand, LCIA methods showed a higher level of regionalization compared to the LCI nomenclature. In this case, a large number of elementary flows referring to watersheds for water flows, ecoregions for land use, or countries for several flow groups were not considered in the “aligned extended method.” In the case of LUIS, the extended method included around 25,000 flows that were reduced to 103 flows due to the lack of spatial resolution in the LCI. A list of elementary flow categories discarded in each LCIA method is provided in Supplementary Material (Table SM4.2), while the comprehensive list of discarded elementary flows can be explored by LCIA method in the mapping document indicated by the mapping rule “NO_MAP” (Supplementary materials 2 and 3).

3.2.2 Level of coverage of mapped methods

The resulting mapped methods covered between 12.5% (ReCiPe) and 100% (LUIS) of the elementary flows of the aligned extended methods (Fig. 4a, Table 5), i.e., the maximum number of elementary flows that could be mapped to the LCI nomenclature. The coverage level largely varied among impact categories (Table SM4.4), with water use (> 99% among different methods) and land use (> 53%, among different methods) showing a high coverage level. Regarding water use, the level of regionalization at the country level in the LCIA methods was aligned to the LCI nomenclature (Table SM4.2). On land use, ReCiPe showed the lowest coverage level (53%) compared to the other methods (> 64%) (Table SM4.4) as the considered impact assessment model addresses a more limited number of land use categories, namely only land transformation to and from natural land (i.e., non-use situation) is considered in the calculation of transformation impacts.

On the contrary, toxicity and climate change impact categories had a narrower coverage among the different methods. Among those methods considering also toxicity impact categories, coverage was mainly determined by the low coverage of chemicals in toxicity categories, which ranged between 6% (Human toxicity, carcinogens in Stepwise 2013) and 39% (Human toxicity non-cancer, long term in Impact World+) (Table SM4.4). Toxicity-related categories represented the ones with the largest share of elementary flows in these methods (> 50% of elementary flows), apart

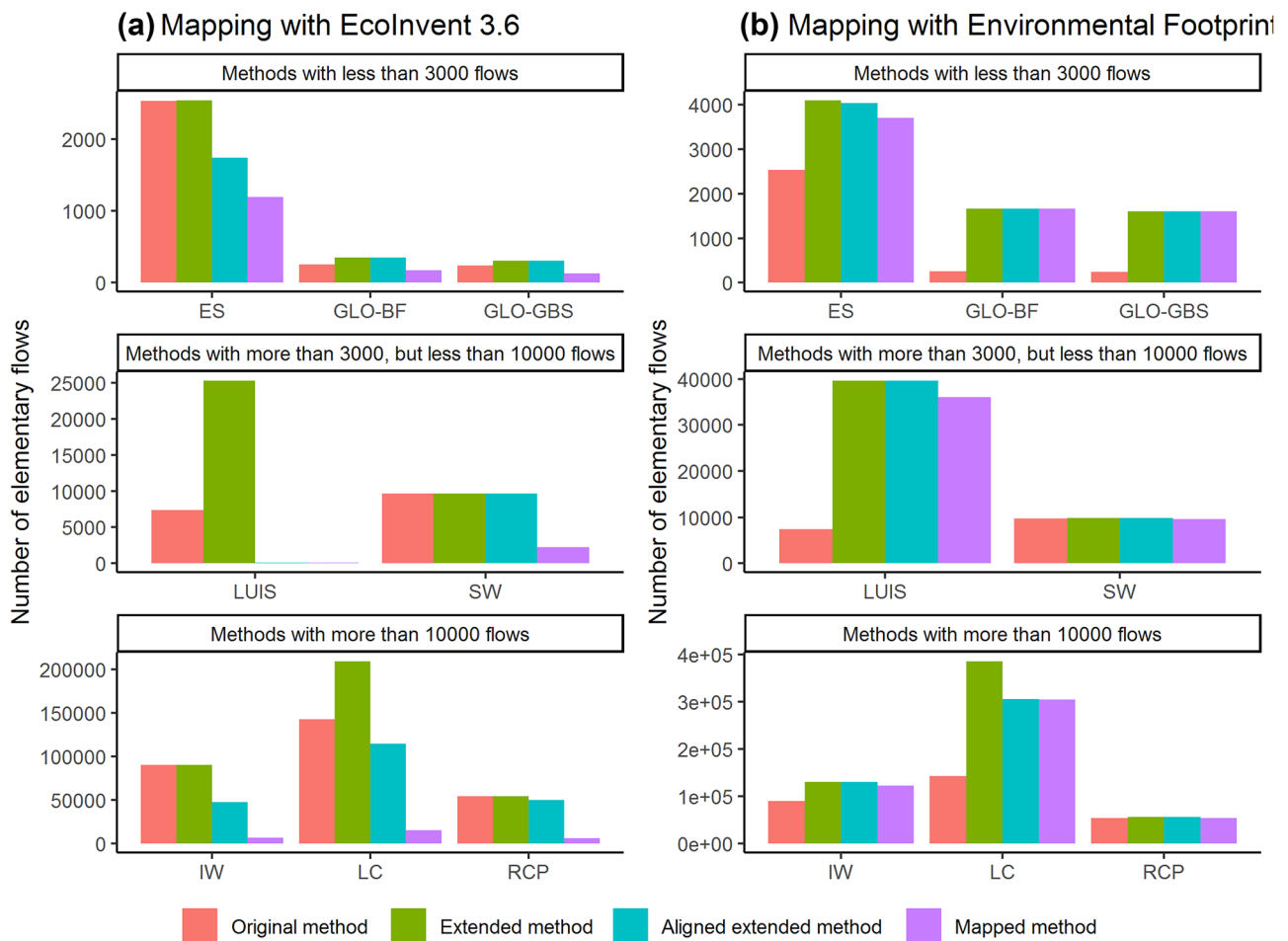


Fig. 4 Number of elementary flows of the original, extended, aligned extended and mapped method: **a** mapping to ecoinvent nomenclature, and **b** mapping to EF nomenclature (Acronyms are explained in Fig. 3)

from Ecological Scarcity (23%) (Fig. 5). The large presence of toxicity-related elementary flows in the methods led to a noticeable effect on the overall coverage of elementary flows at the LCIA method level; e.g., toxicity-related flows may represent more than 85% for methods with limited regionalization (e.g., ReCiPe). In the same line, flows addressed in climate change impact categories were covered between 16% (LC-IMPACT) and 34% (Stepwise). In this case, although LCIA methods and models provided CFs for up to 211 elementary flows (ReCiPe), a limited number of greenhouse gases were available in the LCI nomenclature. In the LCIA methods and models evaluated, mapped flows on climate change ranged from 15 (Ecological Scarcity) to 40 (GLOBIO, both approaches) (Table SM 4.4). In both cases, this was associated to the large coverage of substances in the underpinning impact assessment models (e.g., IPCC in the case of climate change). While LCIA methods and models can address a larger number of substances, there is still a limited coverage and level of detail regarding chemicals and greenhouse gases in LCI nomenclatures. Finally,

LCIA methods also included other substances present in the SimaPro software that were not available in the LCI nomenclature, as these were used by other LCI databases (e.g., Agrifootprint, USLCI) rather than ecoinvent (detailed information provided in Supplementary materials 2).

3.3 Analysis of uncharacterized flows

The assessment of a case study (Step 4) allowed analyzing the uncharacterized flows in the case of LCIA methods. Stepwise (2259 flows) and Ecological scarcity (1780 flows) were the methods that resulted in more uncharacterized flows after running the case study (Table 5). Note that the analysis was performed at the elementary flow level (i.e., considering the context (compartment, subcompartment) rather than at the substance level. Uncharacterized flows were classified according to their typology (Fig. 6, Table SM 4.5), outlining that most of them were under the categories “Chemical organic” (between 19 and 20%), “Raw material” (between 17 and 29%), “Chemical, inorganic”

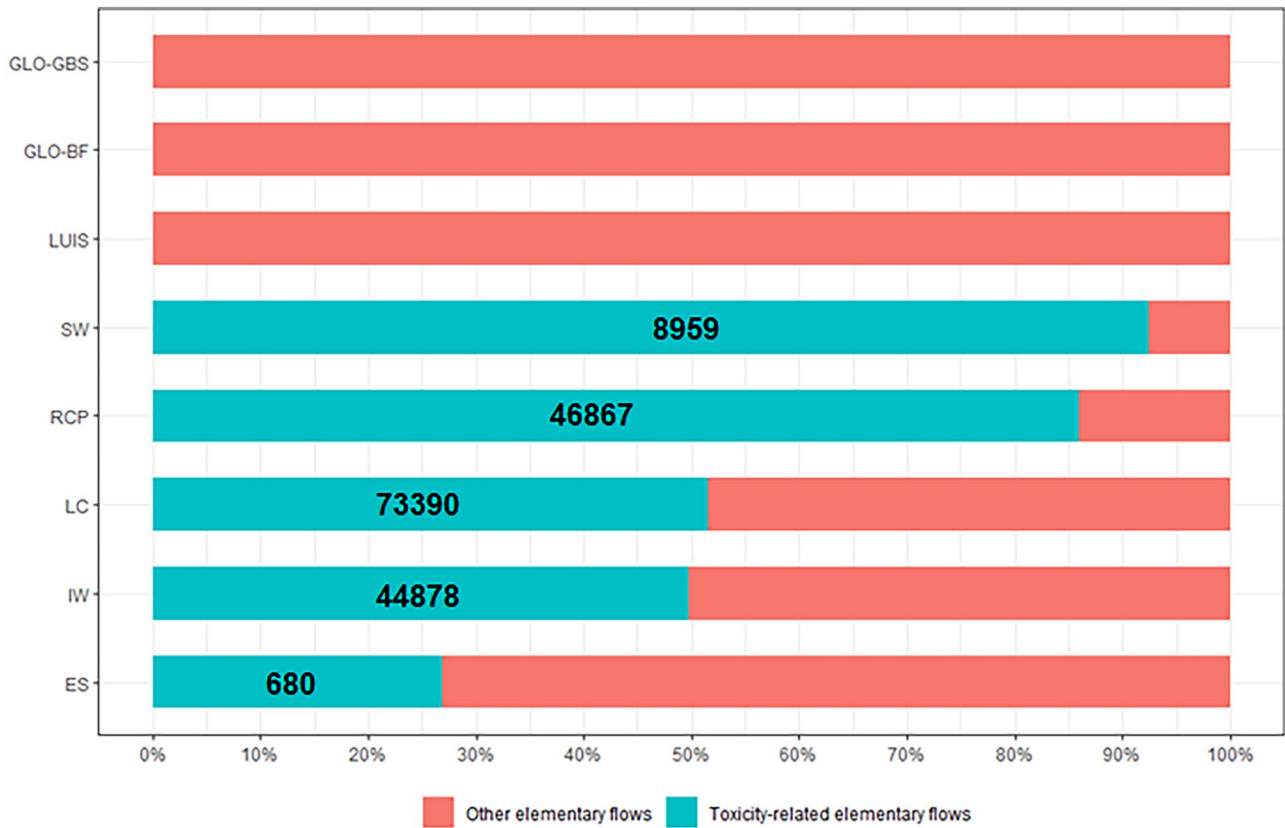


Fig. 5 Share of toxicity-related elementary flows compared to overall elementary flows (acronyms are explained in Fig. 3). Number of toxicity-related elementary flows are reported in the blue bar

(between 9 and 18%) and “Chemical radioactive” (between 9 and 14%). Chemical groups were relevant for “Chemical organic, groups,” which represented between 4 and 8% of

the uncharacterized elementary flows. This indicates that further efforts in LCIA modelling should consider a better coverage of these type of flows. In the context of impacts on

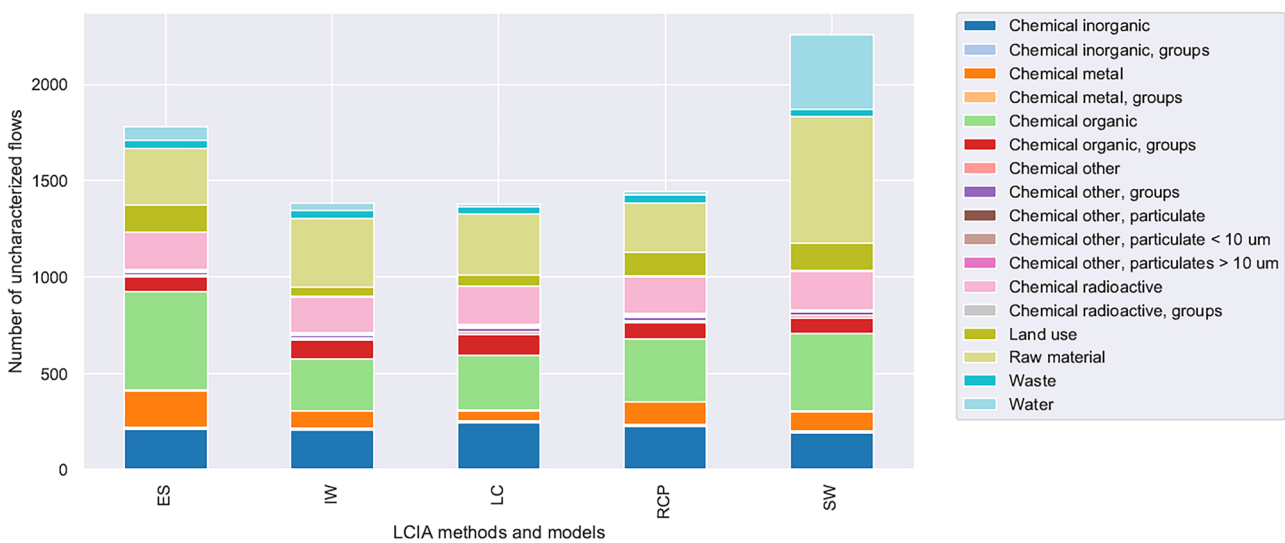


Fig. 6 Share of uncharacterized flows of the analyzed case study (Step 4), by substance type and LCIA method (acronyms are explained in Fig. 3)

biodiversity, attention should be paid to organic, inorganic, and radioactive chemicals, as raw materials contribute to a different AoP at the endpoint level. This is in line with the limited coverage observed of elementary flows in toxicity-related impact categories among the different LCIA methods. In the case of Stepwise, the number of “Water” flows left uncharacterized had a larger relevance (18%) compared to the other LCIA methods as water use is not included as impact category (Table SM1.1). Regarding land use flows, land transformation was more relevant (80%) than land occupation, since some methods only covered land occupation (e.g., Ecological Scarcity) or had a limited coverage of land transformation (e.g., ReCiPe). A total of 977 flows were uncharacterized in the five LCIA methods, highlighting common gaps in the coverage of chemical organic (20%), raw materials (20%), chemical radioactive (17%), chemical inorganic (17%), and chemical metal (5%).

3.4 Comparison with the mapping to the Environmental Footprint nomenclature

The LCIA methods and models were also mapped to the EF 3.0 nomenclature (Supplementary material 3) for comparative purposes. Regarding the EF 3.0 nomenclature, the coverage of flows was larger than for ecoinvent LCI nomenclature, ranging from 91.6% (ES) to 99.6% (GLOBGS) (Table 5), due to the following: (a) the larger number of elementary flows regarding chemicals and greenhouse gases (Table SM4.6) and (b) the higher regionalization of the elementary flows, when compared to ecoinvent. Notwithstanding that regionalization is implemented in the EF 3.0 for water use, land use, eutrophication, and acidification; alignment was only partial since this is limited to the country level (including some flows only for EU countries, such as acidification), thereby excluding different spatial resolutions (e.g., ecoregions, watersheds) in the aligned extended methods (Table SM4.2).

4 Discussion and recommendations

The mapping process followed in this paper required the definition of several mapping rules leading to specific choices often taken in collaboration with LCIA method developers. So far, the mapping of LCIA methods (and models) to LCI nomenclatures has not been subject to the development of a systematic approach. However, with the continuous development of LCIA models and methods and the inclusion of new environmental aspects in LCA, the improvement of the coherence of the LCI-LCIA connection is more and more relevant. Mapping rules addressed aspects present in the LCA literature regarding the following: the definition

of elementary flows (Edelen et al. 2018; Koellner et al. 2013a), interoperability (Suh et al. 2016), LCIA implementation (Hischier et al. 2010), and the LCI-LCIA connection (UNEP 2020).

The mapping process was supported by a mapping tool complemented by a manual mapping, mainly focused on the context and the substance name of elementary flows. In line with previous findings in the literature (Edelen et al. 2018), a lower level of standardization of nomenclature for non-chemical elements or compounds required defining specific mapping rules for groups of elementary flows, namely chemicals, carbon, land use, water, and particulate matter. Regarding substance names, patterns with different levels of detail and order of components employed in the different nomenclatures hampered a smooth identification of corresponding flows. Using different nomenclature patterns in the substance name of elementary flows is more common for land use flows (Edelen et al. 2018), due to multiple levels of regionalization and a lower nomenclature alignment. Although Koellner et al. (2013a) proposed a harmonized nomenclature for defining land use flows, this has not been widely implemented in LCI and LCIA models so far. However, efforts such as for land use flows would be required for the different flow categories, in order to ease the harmonization of nomenclatures in the LCA community.

The inclusion of a case study (Step 4 for LCIA methods and mapping to ecoinvent nomenclature) was a key to identify missing flows in the mapping procedure through the analysis of uncharacterized flows. In particular, this step revealed several aspects to be considered in the harmonization of nomenclatures, including synonyms, redundancies, and syntax errors (Edelen et al. 2018). Stakeholders involved in this harmonization quest (LCIA, LCI, and LCA software developers) should take these issues into consideration in the revision of their developments, as they were specially hampering the automation of the mapping process and are prone to generate errors.

Providing the context for an elementary flow is fundamental for LCIA and the different level of detail in terms of context (compartment, subcompartment) were found as a potential source of uncertainty in LCIA results due to value choices taken in the defined mapping rules. In these cases, LCIA developers should consider the full coverage of context categories (compartment-subcompartment) rather than limiting the provision of CFs to specific compartments. Most specifically, the provision of CFs for the “unspecified” subcompartment should be of utmost priority for LCIA developers. Otherwise, LCIA developers should embrace the responsibility of providing specific guidance for the implementation by LCA practitioners, thereby reducing the range of uncertainty for the latter. A harmonized definition of context categories in the LCA community would enhance such practices.

In the same line, a different level of detail was observed for substance names. In general, LCI nomenclatures showed a higher level of detail than LCIA methods and models. A clear example is the categorization of land occupation/transformation or water flows with a higher level of detail in LCI compared to in LCIA, which led to a mapping with flows in a different level of detail. This aspect is linked to the data quality and accuracy in defining elementary flows (Edelen et al. 2018), in which further development is required in LCIA methods. For example, the land use intensity-specific LCIA model evaluated in this study included an additional level of detail for land use flows (i.e., intensity of use), allowing for a better alignment to the resolution of data compiled in LCI databases. For example, different levels of detail in land use nomenclature affected the ranking of most contributing food products in an EU-wide case study (Crenna et al. 2019).

On the other hand, limited development of LCI databases can also hamper the full implementation of LCIA methods and models, limiting the robustness of the results. This was observed for two main aspects: the larger presence of elementary flows in LCIA methods than in LCI nomenclatures (e.g., chemicals, greenhouse gases) and the level of regionalization. While LCIA methods are increasing the number of elementary flows for which CFs are provided by enlarging the coverage of substances, the expansion of elementary flows in LCI databases might require additional work to incorporate them, thereby increasing data quality and accuracy (Edelen et al. 2018). However, this task might demand a large effort and targeting key elementary flows (i.e., prioritizing) according to their environmental impact relevance that could support the definition of improvement needs.

Regionalization has rapidly evolved in the LCA community, mainly focusing on LCIA development and specific software to perform regionalized LCAs (e.g., Brightway) (Mutel 2017). The limited spatial resolution of inventory data has been highlighted in a recent survey on LCIA regionalization (Mutel et al. 2019). In our results, the addressed LCIA methods included fine spatial resolution, such as terrestrial (Olson et al. 2001), freshwater (Abell et al. 2008), and marine (Spalding et al. 2007) ecoregions. However, LCI nomenclatures showed a very limited regionalization. In the case of ecoinvent, regionalization was limited to water use flows at the country level, although the finest spatial resolution of some LCIA methods was at watershed level. In the case of land use flows in LC-IMPACT, the world-average global CF per land use type was employed in the mapping to the ecoinvent nomenclature although this is recommended to be applied only for elementary flows with unknown location (Verones et al. 2020). Concerning the EF3.0 nomenclature, country-level regionalization was provided for some groups of elementary flows (e.g., land use, water) although

limited to EU countries for some impact categories (e.g., acidification, eutrophication). In this context, LCI nomenclatures currently prevent the implementation of advancements towards a more refined spatial resolution in LCIA methods and models, outlining the necessity for further regionalized inventory data (Mutel et al. 2019). For LCA practitioners aiming at performing analysis at higher resolution and improving the accuracy, the proposed mapping should be complemented, e.g., by adding new elementary flows with the corresponding resolution and forcing its inclusion in the LCI nomenclature (i.e., and thus making it available in the software for its inclusion in the LCI compilation of the case study).

Divergences in the modelling approaches adopted in LCI and LCIA methods were unveiled during the mapping process highlighting the required knowledge for properly mapping LCIA methods and LCI databases with regard to not only impact assessment modelling but also inventory modelling in the specific databases. In the case of LC-IMPACT, land use (Sect. 3.1.4) and water use flows (Sect. 3.1.5) were adjusted to reduce misleading results in the implementation when using the ecoinvent database. Therefore, LCA practitioners might find several difficulties in this endeavor due to the diverse aspects to be considered. Accordingly, multi-stakeholder efforts for agreed and harmonized nomenclatures, from substance name to regionalization levels, are required to marginalize the room for errors in connecting LCIA and LCI nomenclatures.

Based on this study, a number of recommendations to improve the LCIA-LCI connection have been identified, resulting from a collective effort of different stakeholders, as follows:

- The entire LCA community — including LCA software developers, LCIA method developers, and LCI database developers— may:
 - Contribute to the harmonization of substance name (incl. level of detail and nomenclature pattern)
 - Contribute to the harmonization of context definition (compartment-subcompartment naming and structure)
 - Revise further development in light of syntax errors, redundancies, and synonyms (e.g., chemicals)
- LCIA method and LCI database developers may:
 - Increase coverage of chemicals (e.g., uncharacterized flows)
 - Set harmonized rules for chemical names, e.g., deciding on a specific univocal nomenclature
- LCIA method developers may:

- Provide CF for “unspecified” subcompartment or specific implementation guidance
 - Improve the level of detail of substance name (e.g., land use)
- LCI database developers may:
- Increase the coverage of carbon flows
 - Increase the spatial resolution

5 Conclusions

For improving the operationalization of LCIA methods, there is the need of developing a systematic mapping between the nomenclatures adopted in LCI and LCIA. This paper contributes to the operationalization of LCIA methods and models addressing impacts on biodiversity by proposing a mapping process to better connect LCI and LCIA nomenclatures. A mapping is proposed for eight LCIA methods and models and two LCI nomenclatures. A key step to map uncharacterized flows was the implementation of a case study. Furthermore, the case study helped to highlight substance groups in which LCIA modelling should focus further efforts.

The results of this study can support the path towards harmonizing the nomenclature of elementary flows in the LCA community. The results highlight the role of the different stakeholders in this process which would benefit from a harmonization of not only substance names but also the context (i.e., compartment-subcompartment). Due to the different pathways taken in LCIA and LCI development, specific gaps were found identifying a list of recommendations towards a better LCIA-LCI connection. Among the LCA community, LCA software developers are placed in the interface of LCI and LCIA and should also align their implementation to harmonize nomenclatures, particularly when adapting native LCI and LCIA nomenclatures.

The provision of LCI-LCIA mappings agreed with different stakeholders (LCI, LCIA, and LCA software developers) may enhance a wider use of recent LCIA developments by practitioners. For example, Chaudhary and Brooks (2018) included a mapping with the proposed harmonized nomenclature for land use flows (Koellner et al. 2013a), simplifying the mapping with different LCI nomenclatures. To compare and assess different LCIA developments, such as for impacts on biodiversity, flow interoperability among different data sources and methods is fundamental (Edelen et al. 2018). In this pathway, international and multi-stakeholder initiatives are of great relevance, such as the current GLAD and GLAM efforts (Life Cycle Initiative). In both cases, LCI-LCIA connection and interoperability are at the core of specific

working groups and taskforces. While this study was done in the context of LCIA methods and models addressing biodiversity, the relevance of harmonized nomenclatures and mapping efforts is common in LCA and necessary across all impact areas and associated AoPs.

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Declarations

Conflict of interest The authors declare no competing interests.

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