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Effect of software choice and LCI database evolution on a comparative LCA study of permanent magnets

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Abstract

Life cycle assessment (LCA) databases and software evolve. We analyzed to which extent software and evolving life cycle inventory databases affect the comparison of technology alternatives, using a comparative LCA on permanent magnets as a case study, with two selected software tools: CMLCA and Brightway LCA. We migrated the system models from the CMLCA to Brightway LCA software and alternated between the ecoinvent database versions 2.2 and 3.1 to 3.6 in the system background. When using ecoinvent v3.6 instead of v2.2, the change of the indicator results ranged from −34% to 283%. The evolution of the ecoinvent database impacted the absolute amounts of the characterized results and the relative performance between alternatives. The impact category with the highest variability was ionizing radiation, which even showed a ranking inversion with ecoinvent v3.4. In contrast, the impact of using CMLCA or Brightway was negligible because the same data and modeling assumptions caused percentage differences below 0.4%. During the semi-automated data migration to Brightway, we identified 23 environmental flows in the CMLCA model that were not paired with their corresponding characterization factors in the published study of reference. This error had led to an underestimation of 63% in the photochemical oxidation indicator of one of the alternatives. This underestimation relates to an interoperability issue regarding the nomenclature of environmental flows in software alternatives and is a matter of data implementation rather than an issue intrinsic to the selected software. Finally, we identified improvement opportunities for the transparency and reusability of LCA models. This article met the requirements for a Gold-Gold JIE data openness badge described at http://jie.click/badges.

KEYWORDS
background, industrial ecology, interoperability, LCA, LCA software, LCI database

1 | INTRODUCTION

Life cycle assessment (LCA) allows to model the environmental interventions of a product at every stage of its life cycle (ISO 2006). Among various possible applications, this tool has been widely used to guide decisions regarding which alternative product or technology performs better, from an environmental perspective (Guinée et al., 2011; Lin et al., 2019).

Despite the growing popularity of LCA for a growing variety of applications, the outcomes of LCA studies are difficult to reproduce due to factors such as little compatibility between data exchange formats and LCA software, and restricted access to data . Furthermore, Seidel (2016) observed that the adoption of LCA as a supporting tool for policy making has been hindered by unclear communication of modeling assumptions and lack of transparency. The lack of transparency leads to uncertainty regarding the robustness of LCA outcomes and regarding the validity of the underlying data (Guinée et al., 2018). To improve the transparency and accessibility of data in their publications, the *Journal of Industrial Ecology* modified their publication requirements and started a system of optional data openness badges (Hertwich et al., 2018). Adding to that effort, we argue that further compatibility between life cycle inventory (LCI) data formats and attention to the evolution of large LCI databases would enhance the reliability, transparency, and usefulness of LCA studies.

The use of an LCI data format is database and software specific. Many LCA software tools exist, and several articles have investigated the role of software selection as a factor that influences LCA outcomes. The LCA software considered in previous studies included GaBi, SimaPro, openLCA, Umberto, and Quantis Suite. Some studies focused on the comparison of the environmental profile of a set of individual products modeled with different software (Herrmann & Moltesen, 2015; Silva et al., 2019). In contrast, other studies explored the effect of the software selection on comparative LCAs (Seto et al., 2017; Speck et al., 2015, 2016). All the studies observed differences in the indicator results when using different software. The comparative studies even observed ranking inversions.

The experimental designs of these studies started from the premise that the software selection is a variable that might impact the outcomes of an LCA. Later in their analyses, Herrmann and Moltesen (2015), Speck et al. (2016), and Silva et al. (2019) observed that the differences they found were rather rooted in the data implementation. In this context, “data implementation” refers to the process in which the data on unit processes or life cycle impact assessment (LCIA) methods are first transformed from their original formats and then loaded to the LCA software.

Many commercial LCA software packages, such as GaBi and SimaPro, come with preinstalled LCI databases. Here, data implementation of LCI databases and LCIA methods is done by the software providers. By contrast, for some free software such as Brightway and CMLCA, the user is responsible for loading these data into the software environment (Heijungs, 2017; Mutel, 2017). Accordingly, in this study we profited from the user control that Brightway and CMLCA provide. With this control, we tested the hypothesis that the same data and modeling assumptions should yield the same results.

LCI databases themselves are crucial for the outcomes of LCA studies. Large LCI databases provide generic data for the compilation of LCIs in LCAs. These generic data are often used to model the background of a product system.[1] Although an important goal of LCAs is to highlight environmental improvement options in the foreground processes of product systems,[2] their outcomes largely depend on the background processes (Kuczenski, 2019). For instance, Mendoza Beltran et al. (2018) showed how the environmental profiles for the technological development of electric vehicles would change if the secondary data constituting the background electricity processes were changed to make them consistent with future scenarios. In relation, some studies have observed large discrepancies when using LCI databases from different providers (Kalverkamp et al., 2020; Pauer et al., 2020).

LCI databases are expected to offer reliable and realistic representations of the technologies in use. The ecoinvent database, which is popular amongst LCA practitioners, addresses this expectation by maintaining a continuous improvement approach, adhering to quality guidelines, and updating or incorporating LCI datasets (Reinhard et al., 2019; Wernet et al., 2016). Despite the existence of more than a dozen LCI databases, the ecoinvent database remains one of the best valued across LCA practitioners due to its process coverage and perceived transparency (Beemsterboer et al., 2020; Saade et al., 2019; Suh et al., 2016).

Since the launch of version 3.0 of the ecoinvent database, nine minor versions have been released. Although many studies make use of the ecoinvent database, to our knowledge no analysis has been performed on the effect of evolving LCI databases, such as ecoinvent, on the outcome of comparative LCA studies. Yet, it is likely that such effects exist. Steubing et al. (2016) pointed to differences on the life cycle indicator results of equivalent functional units represented in ecoinvent versions 2.2 and 3.0, caused by data updates and the introduction of new modeling principles. They concluded that LCA outcomes will continue to change with the evolution of LCI databases.

Against this background, the objective of our study is to analyze to which extent software and evolving LCI databases affect the comparison of technology alternatives. We used the work by Sprecher et al. (2014) on the primary and secondary production of permanent magnets as a case study. Sprecher's original comparative LCA was modeled in CMLCA and used ecoinvent v2.2 for the background processes. We replicated the analysis in Brightway (Mutel, 2017), using ecoinvent v2.2 (Frischknecht et al., 2005) and the cut-off models of ecoinvent v3.1 to v3.6 (Wernet et al., 2016). We analyzed the differences at the indicator results level and at the interpretation level. Finally, we provide some recommendations to improve the transparency and reusability of LCI datasets.

2 | METHOD

We compared the environmental profiles of permanent magnet production systems, keeping the foreground data constant while changing the LCA software and background data. We selected the case study pragmatically, based on the availability of the product system models in a computer-readable format. We drew recommendations regarding transparency and reusability based on interoperability aspects. In this section we first provide an overview of such aspects, then we present the case study, and finally, we present the quantitative indicators used in the analysis. Every dataset used for the calculation of the quantitative indicators is available in the Zenodo archive at https://doi.org/10.5281/zenodo.7268486.

2.1 | Interoperability of LCI databases and LCA software tools

In the context of the FAIR Guiding Principles for scientific data management, Wilkinson et al. (2016) defined interoperability as "the ability of data or tools from non-cooperating resources to integrate or work together with minimal effort." In the LCA field, the multiplicity of sources of LCI datasets (e.g., LCA studies, LCI databases, and databases from other domain) is a particular case of non-cooperating resources. Another particular case is the existence of multiple LCA software tools with their corresponding data exchange formats.

The following subsections further describe examples of interoperability aspects related to data implementation, grouped into three types of LCA data: LCI databases, LCIA methods, and product system models. Section 2.1.1 illustrates the evolution of LCI databases, focusing on the ecoinvent database. Section 2.1.2 illustrates the evolution of LCIA methods, using CML-IA as an example and drawing from the ecoinvent documentation. Last, Section 2.1.3 focuses on product system models and presents a link between transparency, reusability, and interoperability.

2.1.1 | Evolution of the ecoinvent database

Fritter et al. (2020) proposed the nomenclature and format used in LCI databases as the core criteria for their interoperability. According to this proposal, the ecoinvent database is highly interoperable because more than a dozen LCA software tools are compatible with its nomenclature conventions and its format. However, there are variations in the implementation of this database in the different software tools. For example, it comes preinstalled with other databases in the two leading LCA software tools, SimaPro and GaBi (Herrmann & Moltesen, 2015), and it has to be installed from the XML file in the EcoSpold formats in Brightway and CMLCA.

On average, the ecoinvent Association launches a new version of the ecoinvent database every year. Each new version contains improvements due to the correction of identified errors or due to the incorporation of new data. In this way, the evolution of the ecoinvent database also involves the deletion of outdated unit processes, which become replaced with updated or more representative data (ecoinvent, n.d .). Some of the LCI datasets in the precedent versions have a one-to-one correspondence to the newer versions, with some datasets only undergoing nomenclature changes. For example, the LCI dataset named "nickel, 99.5% at plant" in v2.2 is equivalent to the LCI dataset named "nickel, 99.5%" from the activity "nickel mine operation, sulfidic ore" in v3.0, with no differences in the inputs and outputs connected to the unit process (Moreno-Ruiz et al., 2013). The changes between each version are documented in reports. These reports provide a general explanation of the changes and refer the readers to appended correspondence files for further details on the specific changes.

2.1.2 | Support of LCIA methods

LCIA method refers to a selection of impact categories related to specific characterization models used during the LCIA phase of the LCA framework (Althaus et al., 2010). At the LCIA phase, the inventory of environmental interventions associated with a product system is converted to scores on impact categories like acidification, global warming, and so on. For this, the environmental interventions have to be paired correctly with characterization factors stemming from specific characterization models (ISO. 2006). The LCIA methods also evolve with time. As an example, the remarks tab of the released file for CML-IA v4.8 mention several updates from v2.0, released in 2001, to v4.8, released in 2016. Besides, eight cells contain mentions of mistakes, errors, or corrections addressed between v2.0 and v4.2 (van Oers, 2016).

The ecoinvent database also provides information on its LCI datasets at the level of characterized results. For their calculation, many LCIA methods are implemented in the ecoinvent database. For example, characterized results for many LCIA methods, including CML-IA and ReCiPe (Huijbregts et al., 2017), are available for ecoinvent v3.6 (Moreno-Ruiz et al., 2019). However, in ecoinvent v3.6, the data implementation of the CML-IA method was marked as "obsolete," and as "superseded" in v3.7, which means that the database keeps it for legacy reasons but that it is no longer maintained (Moreno-Ruiz et al., 2019, 2020).

According to Moreno-Ruiz et al. (2019), stopping the maintenance of an LCIA method means that:

TABLE 1 Reference flows evaluated in this study. The labels used in the original study by Sprecher et al. (2014) are indicated within brackets

Functional unit	Alternative
1 kg of Nd-Fe-B magnet	From the primary production of Nd (primary, baseline)
	From short loop recycling (recycled via hand picking)
	From long loop recycling (recycled via shredding)

1. New errors identified in the implementation of unmaintained LCIA methods will not be corrected.
2. Unmaintained LCIA methods are not updated to include elementary exchanges added to the ecoinvent database.

As a result, practitioners using different software packages may be unaware that they use different versions of the same LCIA method. For example, the default setup of Brightway v2.3 installs around 700 sets of characterization factors as implemented in the LCIA methods supported by ecoinvent v3.6 (Mutel, 2014, 2016, 2020). However, the documentation of ecoinvent v3.6 omits the version of the CML-IA method it implements, while the documentation of ecoinvent v2.2 describes it supports v3.3 (Althaus et al., 2010; Moreno-Ruiz et al., 2019). In contrast, SimaPro v9.2 implemented CML-IA v4.8 (PRé, 2022a). This type of information can be retrieved from a variety of locations. For example, we traced it to the documentation of ecoinvent and SimaPro, and to the documentation and code repository of Brightway. SimaPro also updates its supported methods and keeps legacy access to superseded methods (PRé, 2022b). It follows that heterogeneous documentation and support to LCIA methods are challenges when comparing characterized results generated by different software.

2.1.3 | Transparency, interoperability, and reusability

Kuczenski et al. (2018) makes a distinction between datasets and product system models. On the one hand, LCI datasets consist of information related to “elementary or intermediate exchanges, associated with specific industrial processes or activities” (Kuczenski et al., 2018). On the other hand, product system models are structures in which datasets on unit processes are linked together, to represent the life cycle of a product (Kuczenski, 2019; Kuczenski et al., 2018). As argued by Ingwersen et al. (2018), product system models (complete LCA models) are easier to integrate and reuse than individual datasets or fragments.

According to Fritter et al. (2020), OpenLCA Nexus, ecoinvent, and the UNEP GLAD network are leading the adoption of interoperability practices and are platforms to improve the accessibility to LCI datasets.

Some other initiatives worth mentioning are BONSAI and ODYM because these address the possibility of harmonizing and sharing data that comes from different contexts and from the use of different tools such as LCA, material flow analysis, and environmental input output (Ghose et al., 2022; Ghose et al., 2019; Hansen et al., 2020; Pauliuk & Heeren, 2020).

2.2 | Case study

Permanent magnets from Nd-Fe-B, with a typical chemical formula of $Nd_2Fe_{14}B$, are widely used for wind turbines, electric vehicles, robotics, and hard disk drives (ISO, 2020). The study by Sprecher et al. (2014) provides an LCI for the production of rare earth oxides and compared alternative technological routes to produce Nd-Fe-B magnets. We replicated the foreground of the study by Sprecher et al. (2014) and produced different versions of the product system models by linking the foreground to seven versions of the ecoinvent database as background. As the reference study, we used eight impact categories of the CML-IA method baseline[3] and the three reference flows described in Table 1.

In the reference study, the recycling alternatives showed a better environmental performance than the primary production of Nd-Fe-B magnets. For some impact categories, the improvement was larger than one order of magnitude. The main difference between the alternative product systems of Nd-Fe-B magnets is the source of Nd, as depicted in Figure 1. In the product system models, the primary production takes place in China (CN), while the recycling processes take place in Great Britain (GB). The primary production and the long loop recycling have similar processing steps for processing the primary or recovered Nd oxide into magnetic powder and then into Nd-Fe-B magnets. In contrast, the short loop recycling converts the particles of Nd-Fe-B recovered through hydrogen waste processing into new Nd-Fe-B magnets.

2.2.1 | Adjustments to the foreground system

Sprecher et al. (2014) documented another system feature driving the large differences between the environmental performance of the recycling processes and the primary production of Nd-Fe-B magnets in the supplementary information; namely, the source of nickel (Ni) for electroplating.

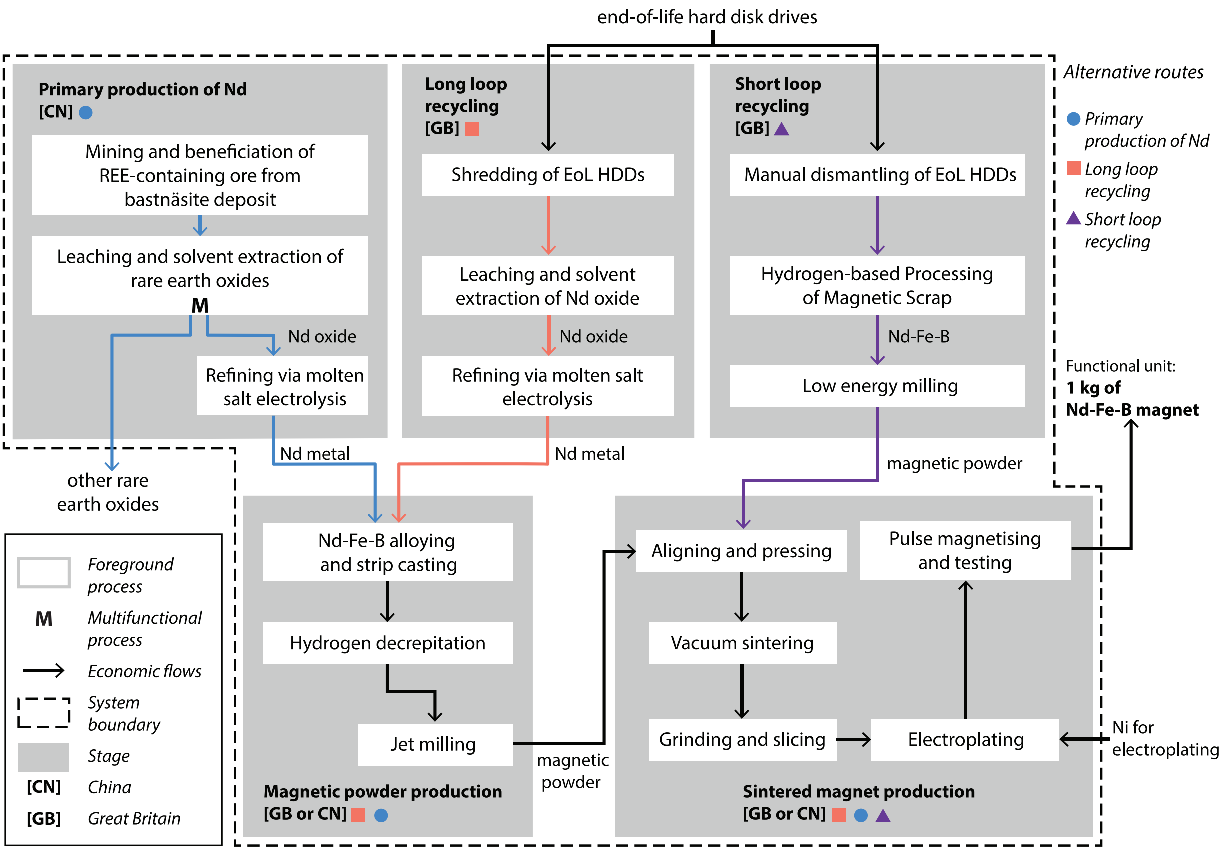

FIGURE 1 Combined flowchart of the production of 1 kg of Nd-Fe-B magnet via three alternative routes.

For the short loop recycling, the original model represented the use of secondary Ni with the LCI dataset "nickel, secondary, from electronic and electric scrap recycling, at refinery" (Classen, 2007). For the long loop recycling and the primary production, the original model represented the use of primary Ni with the LCI dataset "nickel, 99.5%, at plant" (Classen, 2004).

In contrast to the study of reference, we used primary Ni in the product system models of the three Nd-Fe-B magnet alternatives with the intention to stress the role of the source of Nd in the comparison of the alternative routes to produce Nd-Fe-B magnets.

2.2.2 | Computer-aided identification of characterization errors

We obtained the original foreground process and allocation data from the corresponding author of Sprecher et al. (2014) in CMLCA format (lca). Then, we performed the adjustment of the source of Ni on CMLCA. We wrote Python scripts for pre-processing the data into a format supported by Brightway. These scripts are available in the associated repository (Miranda Xicotencatl, 2022). The Python scripts allow the adjustment of the source of Ni directly from the pre-processed data of the original model.

During data pre-processing, we realized that 23 environmental flows in the foreground of the original CMLCA model were not paired with their corresponding characterization factors. The reason for this was that the names and classification of these environmental flows were different from the ecoinvent nomenclature, which was used for the rest of the original model (see Table S1 of the Supporting Information). The Python scripts allow the replacement of nomenclature and the correct pairing of environmental flows with characterization factors.

2.2.3 | Overall deviations from the study of reference

We used two approaches to compare the series of outcomes relative to their magnitude. In the first approach, used in Equations (1) and (3), an updated outcome is compared with a reference outcome. Equation (1) aims at indicating the deviation between the modified and corrected model from the study of reference. In Equation (1), the indicator results of the modified model without disconnection errors, $x_{v2.2}$, correspond to the dataset "REM2_2," and the indicator results from the study of reference, $x_{replicated}$, correspond to the indicator results of the dataset

"REM_replicated_2_2." The indicator results in both datasets were calculated in Brightway, with ecoinvent v2.2 and CML-IA v3.3.

$$\text{Percentage change } (\%) = 100 \times \frac{x_{v2.2} - x_{\text{replicated}}}{x_{\text{replicated}}} \quad (1)$$

A second approach is implemented with Equation (2), when comparing the outcomes of the software alternatives, since no obvious baseline can be selected between the two alternatives (Cole & Altman, 2017).

2.3 | Software comparison

The software alternatives were CMLCA version 6.1 (Heijungs, 2019) and Brightway version 2.3 (Mutel, 2017). We compared the effect of using either CMLCA or Brightway on the LCA outcomes using ecoinvent version 2.2 for all the reference flows, with the adjustment of primary nickel for the electroplating of the three magnet alternatives, as described in Section 2.2.1, and keeping the characterization errors described in Section 2.2.2.

As a basis for comparison, we used two groups of indicators: 2138 characterization factors of the software implementations and the indicator results of the eight impact categories assessed. The differences were measured as the percentage difference of the indicators (Cole & Altman, 2017), according to Equation (2). The indicator results of the model using CMLCA, x_{CMLCA}, correspond to the "CMLCA" dataset, and the indicator results using Brightway, x_{bw}, correspond to the indicator results of the "REM_unlinked_2_2" dataset.

$$\text{Percentage difference } (\%) = 100 \times \frac{\left| x_{\text{CMLCA}} - x_{\text{bw,ref}} \right|}{\frac{x_{\text{CMLCA}} + x_{\text{bw,ref}}}{2}} \quad (2)$$

2.4 | Comparison with evolving versions of the ecoinvent database

We compared the effects of using different ecoinvent versions on the indicator results calculated in Brightway by migrating the background of the modified and corrected model, "REM2_2,", from ecoinvent v2.2 (Frischknecht et al., 2005), to versions 3.1, 3.2, 3.3, 3.4, 3.5, and 3.6 (Wernet et al., 2016).

To compare the outcomes using ecoinvent v2.2 with the outcomes of the most recent version considered (v3.6), the differences were represented by the percentage change of the indicator results, with the same approach as in Equation (1), according to Equation (3). The indicator results of the model using ecoinvent v3.6, $x_{v3.6}$, correspond to the "REM3_6" dataset, and the reference values using ecoinvent v2.2, $x_{v2.2}$ correspond to the indicator results of the "REM2_2" dataset.

$$\text{Percentage change } (\%) = 100 \times \frac{x_{v3.6} - x_{v2.2}}{x_{v2.2}} \quad (3)$$

To illustrate how the evolution of the ecoinvent database could impact the comparison of the alternatives at the interpretation level, we calculated the comparative advantage of each alternative over the worst performer for every impact category and ecoinvent version, according to Equation (4). For each version, impact category, and functional unit, the alternative with the worst performance was the one which scored the highest indicator result ($x_{\max}$).

$$\text{Advantage over the worst performer } (\%) = 100 \times \left(\frac{x_{\max} - x}{x_{\max}} \right) \quad (4)$$

3 | RESULTS

3.1 | Deviations from the study of reference

As Section 2.2 explains, we made two modifications to the product system models of the study of reference before comparing the effect of the LCI database evolution. Figure 2 shows the percentage change of the characterized results of the reference flows. The short loop recycling alternative shows the largest differences; mostly larger than 100%. The impact category with the largest percentage change was photochemical oxidation for all the alternatives.

The large differences for the short loop recycling alternative are mainly due to the substitution of the Ni source for the electroplating process, using a primary source of Ni instead of a secondary source. This substitution is a deliberate modification to the model, which enhances the visibility of the source of Nd.

Impact categories	Primary production	Long loop recycling	Short loop recycling	
Photochemical oxidation	5%	8%	63%	532%
Eutrophication	0%	2%	7%	122%
Human toxicity	0%	1%	7%	201%
Climate change	1%	2%	7%	24%
Acidification	0%	1%	6%	544%
Freshwater aquatic ecotoxicity	0%	0%	0%	86%
Stratospheric ozone depletion	0%	0%	0%	68%
Ionizing radiation	0%	0%	0%	14%
	Correction of characterization errors			*Foreground modification*

FIGURE 2 Change of outcomes of the modified and corrected model, from outcomes of the replicated model. The breakdown shows changes caused by correcting characterization errors and by replacing the secondary nickel in the foreground of the short loop recycling alternative. The percentage change was calculated according to Equation (1).

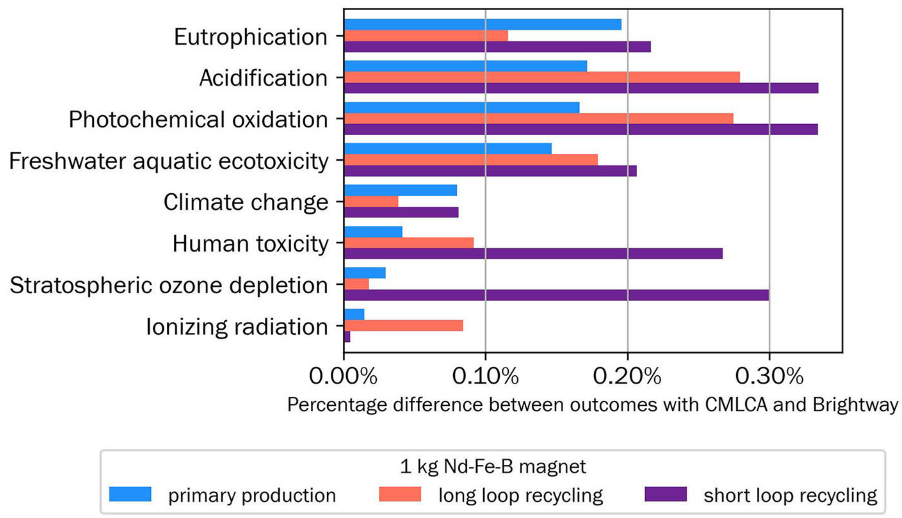

FIGURE 3 Software comparison. Percentage difference between the CMLCA model and its replication in Brightway, calculated according to Equation (2). The underlying data for this figure can be found via the Zenodo data repository at https://doi.org/10.5281/zenodo.7268486.

Smaller differences were observed when correcting the characterization of environmental flows. The error in the original study had led to an average underestimation of about 6% in the indicator results, with a maximum underestimation of 63% in the photochemical oxidation indicator of short loop recycling (see Figure 2). Although smaller in magnitude, this occurrence exemplifies how mismatched nomenclature may lead to characterization errors. Previously, Ingwersen (2015) had reported other instances of mismatched nomenclature leading to characterization errors.

3.2 | Impact of the LCA software tool

At the level of the LCIA method, the environmental exchanges and their characterization factors used in CMLCA and Brightway proved to be the same or very similar. Every environmental exchange characterized in CMLCA was matched to an environmental exchange in Brightway. Besides, the percentage differences between the characterization factors for human toxicity, freshwater aquatic ecotoxicity, photochemical oxidation, and ionizing radiation were below $2.2 \times 10^{-14}\%$ (see Table S2 of the Supporting Information). No differences were found between the characterization factors for acidification, climate change, eutrophication, and stratospheric ozone depletion. At the level of characterized results, the percentage differences between the CMLCA model and its replication in Brightway were below 0.4%, as Figure 3 shows.

The distribution of the small differences found during the software comparison bears no resemblance with the much smaller differences between the characterization factors implemented in CMLCA and Brightway. It may be the case therefore that the differences in Figure 3 are related to differences in the underlying calculation algorithms of each software (Heijungs, 2017). This might be addressed in future research by modifying

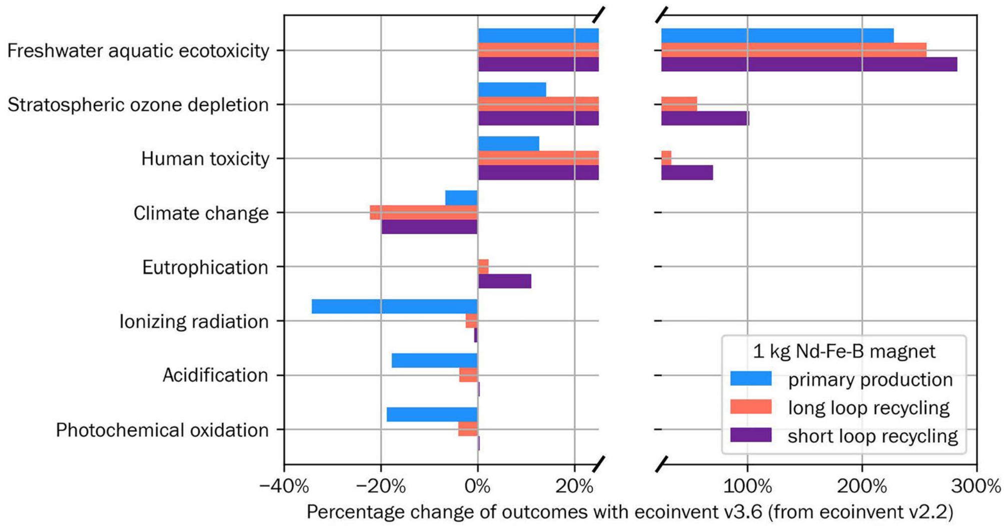

FIGURE 4 Change of outcomes with ecoinvent v3.6 from outcomes with v2.2. The percentage change was calculated according to Equation (3). The underlying data for this figure can be found via the Zenodo data repository at https://doi.org/10.5281/zenodo.7268486.

the calculation algorithm. However, the Brightway documentation does not specify how to do so. Keeping in mind the magnitude of the differences observed, the replication confirmed that the same data and modeling assumptions would yield the same or very similar results in Brightway and CMLCA.

3.3 | Impact of the evolution of the ecoinvent database

3.3.1 | Differences between v2.2 and v3.6

As shown in Figure 4, the choice of ecoinvent version largely impacted the environmental profiles of the alternatives. When using ecoinvent v3.6 instead of v2.2 in the background of the product system models, the indicator results either increased or decreased depending on the impact category and alternative. In five impact categories, the direction or the change was the same within the same impact category; for example, the indicator result for freshwater aquatic ecotoxicity increased for the three alternatives when using v3.6 instead of v2.2. The magnitude of the changes ranged from −34% to 283%. The alternatives scored the largest change on freshwater aquatic ecotoxicity.

The increments or decrements between the outcomes with ecoinvent v2.2 and v3.6 were discontinuous; with no indication of an increasing or decreasing trend along the evolving ecoinvent versions (Figure S1 of the Supporting Information).

3.3.2 | Comparative assessment across versions

Figure 5 shows how the comparative advantages changed with the evolution of the ecoinvent database. For most impact categories, the primary production of Nd-Fe-B magnets remained as the worst performer of the comparison. The long loop recycling was the worst performer for most of the ecoinvent versions on ionizing radiation.

The evolution of the ecoinvent database not only impacted the absolute amounts of the characterized results (see Figure S1 of the Supporting Information); it also impacted the relative performance between alternatives. Although the ranking of preferable alternatives remained constant for most impact categories, the advantages of the recycled Nd-Fe-B magnet alternatives decreased when using ecoinvent 3.6; most notably for freshwater aquatic ecotoxicity.

Ionizing radiation was the impact category with the highest variability, even showing a ranking inversion when using ecoinvent v3.4. Other impact categories with major changes compared to the indicator results of the alternatives with ecoinvent v2.2 are freshwater aquatic ecotoxicity and human toxicity (Figure S1 of the Supporting Information). Below, we analyze the causes behind the aforementioned behavior of these impact categories. Due to the non-trivial effort of tracking changes in the documentation of the ecoinvent database, we decided to limit our contribution analysis to the three impact categories whose characterized results changed the most between ecoinvent v2.2 and v3.6. The ranges of these variations are better illustrated by Figure S1 of the Supporting Information than by Figure 5.

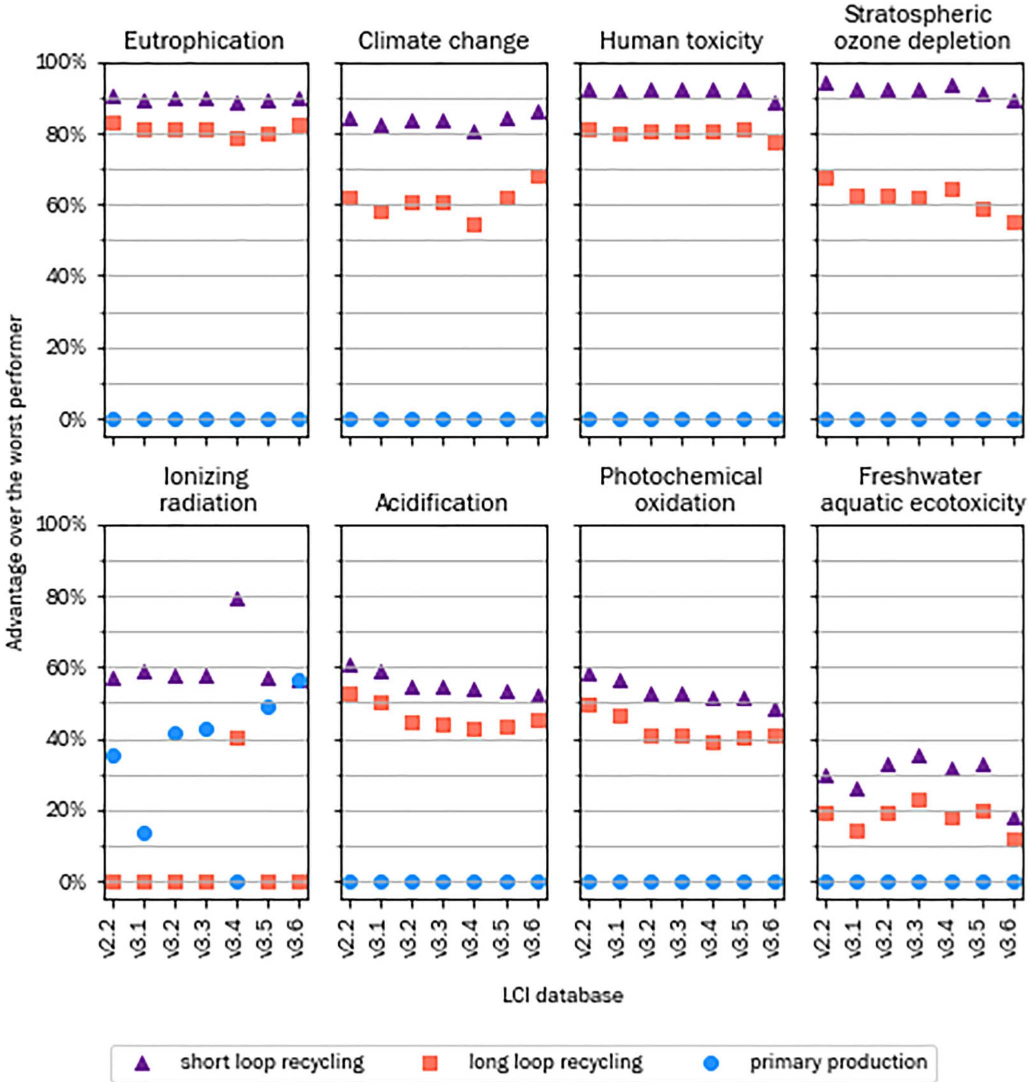

FIGURE 5 Change of environmental advantages with evolving versions of the ecoinvent database. The advantage over the worst performer was calculated according to Equation (4). The functional unit is 1 kg of Nd-Fe-B magnet. The underlying data for this figure can be found via the Zenodo data repository at https://doi.org/10.5281/zenodo.7268486.

3.3.3 | Contribution analysis

Freshwater aquatic ecotoxicity

The magnet production stage, with common processing steps for the three alternatives, largely contributes to freshwater aquatic ecotoxicity. In particular, the Ni for electroplating is responsible for at least 40% of the freshwater aquatic ecotoxicity result for each of the three alternatives when using ecoinvent v2.2. When using ecoinvent v3.6, the contribution of the Ni for electroplating to this impact category grows to at least 73% for every alternative. We traced the reason of this change, further upstream in the production of Ni, to the LCI dataset "disposal, sulfidic tailings, off site." This LCI dataset also appears in the background of the primary production of Nd.

The model for the LCI dataset "disposal, sulfidic tailings, off site" in ecoinvent v2.2 was replaced in ecoinvent v3.6. The replaced model conservatively represented one generic global disposal (Classen et al., 2009). The new and more detailed model generated 43 LCI datasets according to scenarios for seven metal ores in 18 countries and for one generic global disposal (Doka, 2018; Moreno-Ruiz et al., 2019). This model replacement caused the large increment observed in Figure 4 and Figure S1 of the Supporting Information.

Ionizing radiation

The disposal of radioactive waste in the background processes is mostly responsible for the indicator on ionizing radiation. For the alternative using primary Nd, the disposal of radioactive waste is associated to the foreground processes "Mining and beneficiation of REE-containing ore from bastnaesite deposit" and "Leaching and solvent extraction of REOs." This association happens through the upstream use of diesel and kerosene in the background. In the recycling product systems, the disposal of radioactive waste is associated to the share of nuclear energy in the British electricity mix. The rank inversion observed in ionizing radiation with ecoinvent v3.4 (see Figure 5) is caused by the unintended disconnection of the British nuclear production in the activity "market for electricity, medium voltage [GB]," which was reported as a known issue in ecoinvent v3.4. This unintended disconnection also caused an increment in the climate change indicators for the recycling alternatives and was fixed in ecoinvent v3.5 (Moreno-Ruiz et al., 2018).

Human toxicity

The advantage in human toxicity of the recycling alternatives over the alternative using primary Nd remains above 70% with all the ecoinvent versions considered (see Figure 5). The main contributor to this impact category is the primary production stage and then electroplating. In this impact category, the relative performance between alternatives variates little from ecoinvent v2.2 to ecoinvent v3.5. However, the update of the models for disposal of sulfidic tailings, in the background of electroplating, produced a noticeable change in the human toxicity indicator from ecoinvent v3.5 to v3.6. In this sense, the cause of the increment in human toxicity is the same as in freshwater aquatic ecotoxicity but with different magnitudes.

4 | DISCUSSION AND CONCLUSION

As far as we are aware, this is the first study that compared software and versions of LCI databases and identified improvement opportunities within the context of the FAIR data guidelines. The strengths of this study are the computer-aided migration of a foreground dataset from CMLCA to Brightway and the semi-automatic linking of the foreground and the background, using seven different versions of ecoinvent. Besides, the foreground processes can be imported into Brightway and, with access to the ecoinvent database, the entire model can be reproduced. Since the LCI datasets are also provided in a format compatible with Brightway, the characterized results can be recalculated even without access to the ecoinvent database.

4.1 | Impact of the software and the evolution of the LCI databases

In this study, we confirmed the suitability of comparing the characterized results from the LCIA methods implemented in CMLCA, by Sprecher et al. (2014), and in Brightway v2.3, by the Brightway developers. According to the results in Section 3.2, both implementations correspond to CML-IA v3.3, as provided by ecoinvent (Althaus et al., 2010; Moreno-Ruiz et al., 2019). However, we also noted that this version of the CML-IA method is outdated (see Section 2.1.2). When comparing SimaPro and GaBi, Herrmann and Moltesen (2015) also reported difficulties when identifying versions of some LCIA methods implemented and reported the version of the software they used instead. When the version of the LCIA method was unavailable, they would assume that the non-expert LCA practitioner would expect equally updated versions in both software tools. Therefore, the unfulfilled expectation should become clear to all types of LCA practitioners.

The effect of the version of the LCI database was expected to be larger than the effect of the software choice. In fact, the differences resulting from the software comparison were smaller than the differences resulting from the comparison of the evolving LCI database. Figure 6 proposes a classification of the causes of the changes of the indicator results due to the evolution of LCI databases, based on the causes identified in our case study.

Unexpectedly, we found that mismatched nomenclatures within the CMLCA setup of Sprecher et al. (2014) led to erroneous pairing of LCIA methods and environmental flows within the same software. This finding corroborates the observations by Fritter et al. (2020), who suggested that mismatched nomenclatures could potentially result in missing links. This type of errors may potentially propagate to other software setups when exporting data, as we caught in the process of migrating the models from CMLCA to Brightway. Thus, the unmapped diversity of nomenclature in LCA software alternatives can represent a significant barrier to interoperability, impacting the accuracy and comparability of LCA results across different software tools.

As reported in Sections 2.1.1, 2.1.2, 2.2.2, 3.1, and 3.3.3, previous instances of errors in LCI datasets and data on characterization and normalization factors have been reported before. Unfortunately, there are no indications of the magnitude and direction in which errors and future changes in the background LCI databases could impact the environmental profile of a product system. More importantly, it is uncertain how these changes could impact the conclusions drawn from an LCA.

In our case study on the comparison of alternative technologies, the effect of errors in ecoinvent v3.4 caused a ranking inversion of the alternatives on ionizing radiation. In contrast, the change of database version impacted the magnitude of the advantages between the alternatives but not their ranking.

It is worth noting that, for most of the impact categories, the more advanced the applied version of the ecoinvent database was, the smaller was the environmental advantage of the best performing alternative. This result is relevant when reusing LCI datasets without considering the impact

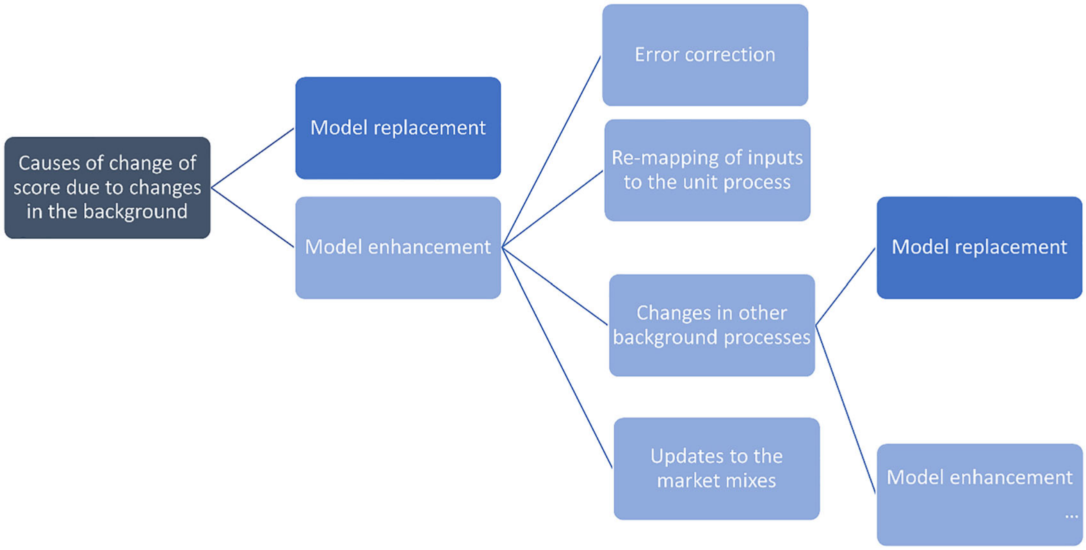

FIGURE 6 Causes of change of indicator results due to changes in the background.

of the background. When the outcomes of a comparative LCA are used for decision support, neglecting the effect of the background could yield to a mistaken recommendation of one alternative over another.

4.2 | Transparent datasets are not enough to ensure interoperability

Transparency that allows reusing data does not imply interoperability. The process data of Sprecher et al. (2014) has been reused in further studies on rare earth production (Bailey et al., 2020; Vahidi et al., 2016). While the data could be manually introduced to software other than CMLCA, the format in which the supplementary data was originally published lacks interoperability with any other LCA software. Although two programs may be compatible with a same format, as for instance CMLCA and Brightway are with EcoSpold, migrations usually require mapping files that are not always accessible to the LCA practitioner. Improving the interoperability of LCI datasets can save time and reduce the risk for misinterpretation and human error. Interoperability facilitates reproduction, re-evaluation, and scrutiny of LCA studies—activities that are the heart of science.

4.3 | Limitations and further research

Our study focuses on the effect of LCA software tools and evolving LCI databases rather than on the technologies compared in the reference study. Nevertheless, our analysis could also inform the development of the compared alternatives to produce Nd-Fe-B magnets. In that sense, we refocused the comparison between the alternative product systems on the source of Nd by harmonizing the source of Ni for electroplating. Besides, we updated the calculated environmental profiles by using more recent versions of ecoinvent to represent background processes. However, the reach of these updates for the comparison of these technologies is limited by the foreground data. For example, Marx et al. (2018) and Bailey et al. (2020) provide more recent data on the primary production of REOs from different deposits and Karal et al. (2021) performed an ex ante LCA on a technology similar to the long loop recycling depicted here.

Since this study was limited to the identification and replacement of strings for the data migration across the versions of ecoinvent, a comparison of the characterized results, using different versions of ecoinvent in CMLCA, is beyond our intended scope. Currently, it is only possible to import a Brightway model in CMLCA manually.

Although we mentioned previous observations of large discrepancies when using LCI databases from different providers (Kalverkamp et al., 2020; Pauer et al., 2020), our study is limited to the implementation of the ecoinvent database in two software alternatives. Further research on the preponderance of interoperability issues could guide efforts to expand the coverage of effects caused by diverse LCI databases and diverse software.

Some possible directions of future research are outlined next:

- Others could use this research by mapping other software and allowing round trips of the models and data between the software alternatives.
- Future research on backgrounds should be done for a systematic approach to future scenarios.

- Future research could consider the role of the algorithms used for the calculation of the environmental profile.

4.4 | Recommendations

LCA practitioners could improve the reproducibility of their research outcomes in open software and prepare their models to face the evolution of LCI databases in the following ways:

- Submitting datasets to well documented and well maintained databases or repositories. The repositories could be specialized, like ecoinvent and other nodes connected to the UNEP GLAD network or, generic, like Zenodo.
- Reporting all the relevant metadata for an adequate implementation. The metadata should contain which LCIA method, LCI database, and software package were used, and it should include the version of each of these elements.
- Reflecting on the level at which the models could be reproduced in open software. Some guidelines could be found by following the ongoing discussions on data FAIRness fostered by the UNEP GLAD network, or the BONSAI and ODYM initiatives.

4.5 | CONCLUSION

This study reframes the matter of LCA software comparison into a matter of differences in data implementation and investigates the impact of evolving LCI databases on the results of comparative LCAs. We illustrated that LCI databases and LCIA methods evolve and that the documentation about the implementation of such data is heterogeneously reported. Our comparison between CMLCA and Brightway supports the argument that the same data and modeling assumptions should yield the same results, although potential differences related to underlying algorithms were left unexplored. Our results demonstrated that the comparison of alternative environmental profiles can be influenced by the version of LCI databases. Our analysis also illustrates how transparent reporting and interoperability enhances the reproducibility of LCA results. Thus, this study provides a solid basis for addressing the potential effects of the evolution of LCI databases used in the background of LCA comparative studies.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that supports the findings of this study is described in the supporting information of this article. Most of the data required to reproduce the models described in the manuscript are available in Zenodo at https://doi.org/10.5281/zenodo.7268486. Some of the data that support the findings of this study are only available from ecoinvent. Restrictions apply to the availability of these data, which were used under license for this study.

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NOTES

[1] Guinée et al. (2002) define the background system/process as "a system for which secondary data, viz. databases, public references, estimated data based on input-output analysis, are used in an LCA."
[2] Guinée et al. (2002) define foreground system/process as "a system or process for which primary, site-specific data are used in an LCA, for whatever reason."
[3] Eutrophication, acidification, photochemical oxidation, climate change, ionizing radiation, freshwater aquatic ecotoxicity, stratospheric ozone depletion, and human toxicity (Guinée et al., 2002).

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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