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Auteurs: Authors:	Maxime Agez, Elliot Muller, Laure Patouillard, Carl-Johan H. Södersten, Anders Arvesen, Manuele Margni, Réjean Samson, & Guillaume Majeau-Bettez
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Correcting remaining truncations in hybrid life cycle assessment database compilation

Maxime Agez, Elliot Muller, Laure Patouillard, Carl-Johan H. Södersten, Anders Arvesen, Manuele Margni, Réjean Samson, Guillaume Majeau-Bettez

Abstract

Hybrid Life Cycle Assessment (HLCA) strives to combine Process-based Life Cycle Assessment (PLCA) and Environmentally Extended Input Output (EEIO) analysis to bridge gaps of both methodologies. The recent development of hybrid LCA databases constitutes a major step forward in achieving complete system coverage. Nevertheless, current applications of HLCA still suffer from issues related to incompleteness of the inventory and data gaps: (1) hybridization without endogenizing the capital inputs of the EEIO database leads to underestimations; (2) the unreliability of price data hinders the application of streamlined HLCA for processes in some sectors; (3) the sparse coverage of pollutants in multiregional EEIO databases limits the application of HLCA to a handful of impact categories. This paper aims at offering a methodology for tackling these issues in a streamlined manner, and visualizing their effects on impact scores across an entire PLCA database and multiple impact categories. Data reconciliation algorithms are demonstrated on the PLCA database ecoinvent3.5, and the multiregional EEIO database EXIOBASE3. Instead of performing hybridization solely with annual product requirements, this hybridization approach incorporates endogenized capital requirements; demonstrates a novel hybridization methodology to bypass issues of price unavailability; estimates new pollutants to EXIOBASE3 environmental extensions; and thus yields improved inventories characterized in terms of 13 impact categories from the IMPACT World+ methodology. The effect of hybridization on the impact score of each process of ecoinvent3.5 varied from a few percentages to three-fold increases, depending on the impact category and the process studied, displaying in which cases hybridization should be prioritized.

1. Introduction

1.1 Recent progress in hybrid LCA

There are two main techniques to quantify life cycle elementary flows (i.e., the release of emissions to, and use of resources from, the environment) and their impacts: process-based Life Cycle Assessment (PLCA) and Environmentally Extended Input Output Analysis (EEIO). Both have their respective strengths and weaknesses. PLCA can model the value chain of specific products but suffers from truncation as it necessarily excludes processes from the system boundaries (Majeau-Bettez, Strømman, & Hertwich, 2011; Nakamura & Kondo, 2002; Perkins & Suh, 2019; Pomponi & Lenzen, 2017; Suh et al., 2004). Therefore, the life cycle inventory (LCI) is likely to be underestimated, potentially leading to erroneous conclusions in a comparative PLCA (Lenzen & Treloar, 2003). EEIO does not exclude any inputs from the economy , but it only operates at an aggregated level (by industrial sectors), making it impractical for product-oriented analyses (Miller & Blair, 2009). Hybrid LCA (HLCA) was designed by combining both techniques, each complementing the weakness of the other (Bullard et al., 1978). Process-based LCIs are complemented with EEIO data bringing completeness to PLCA (tiered and integrated hybrid approaches) while EEIO sectors can be disaggregated using PLCA data bringing more specificity to EEIO (matrix augmentation and path exchange approaches) (Crawford et al., 2018). HLCA should thus theoretically solve the truncation problem of PLCA while still allowing the study of specific product value chains. Current HLCAs based on the tiered hybrid approach (THLCA), however, still fail to completely solve the truncation issue of PLCA, as the majority of them rely on truncated PLCA databases to model the generic value chains (background processes) that are not specific to the system under study (foreground). This issue has been highlighted in literature which has repeatedly called for the compilation of THLCA databases (Bontinck et al., 2017; Crawford et al., 2018; Majeau-Bettez et al., 2011; Strømman et al., 2009)), i.e., entire PLCA databases where each process description is completed with EEIO data to mitigate truncation errors. Such THLCA databases have recently emerged thanks to efforts to streamline and semi-automate the hybridization process (Agez et al., 2020; Yu & Wiedmann, 2018). The streamlining enables the hybridization of thousands of processes while respecting a set of rules to ensure the two datasets are reconciled in a coherent manner. By estimating process requirements that had been ignored in the PLCAs, the current existing THLCA databases increased the average Global Warming Potential (GWP100) impact score of cradle-to-gate processes by 14% to 32% compared to the non-hybridized version of the same database. Despite this improved completeness, THLCA databases may still suffer from multiple limitations leading to some remaining underestimations of elementary flows (Agez et al., 2020), namely (1) the non-endogenization of capital goods, (2) the inability to hybridize certain value chains due to the absence of reliable price data to convert monetary flows into physical flows, and (3) the limited coverage of environmental extensions in Multi-Regional Input Output (MRIO) tables. This article aims to tackle these three issues, which are detailed hereafter.

1.2 Capital goods in PLCA, IO and THLCA

A capital good is a good used in the production of products and services that outlives this production process (e.g., factories, computers, machines). Specifically, in national accounts where product flows are computed on a yearly basis, capital goods are defined as “produced assets which are used repeatedly or continuously in production for more than one year” (European Commission, 2008). In 2007, capital goods formation was responsible for 24% of the total GHG emissions worldwide (Södersten et al., 2017). Yet, how to account for these impacts with a life-cycle perspective is not uniform across methodologies.

In PLCA, capital inputs are entered as direct inputs in unit process inventories, as a “unit” of capital good divided by the estimated total output that unit of capital good will help produce during its lifetime. That way, each functional unit of a process is allocated the same impacts due to capital formation (producing the capital good, e.g., construction of a building) and consumption (using the capital good, e.g., maintenance). For example, in ecoinvent3.5, a photovoltaic cell production plant is expected to produce 40,000,000m² of photovoltaic cells over its lifetime, and therefore the production of each m² of photovoltaic cell is ascribed a small fraction (4e-7) of this plant’s production impacts. The underlying assumption in PLCA is that each functional unit is equally responsible for the initial production of the required capital good.

In IO, capital goods are separated from the manufacture of products/services, i.e., the formation of fixed assets is included in the final demand while the consumption of fixed assets is included in the value added. In other words, the production impacts of capital goods are not allocated to the products/services whose production use these capital goods, unlike in PLCA. The formation of capital (and its impacts) is computed separately as its own consumption category. To link capital formation (and its associated impacts) to the sectors using them, capital goods must be *endogenized*.

For THLCA, where PLCA and IO are to be mixed, consistency on capital goods accounting is paramount. Yet the issue has been largely ignored by the THLCA literature, while the same issue is already well known in other hybrid approaches (Dixit, 2017; Dixit et al., 2015). In the tiered hybrid database of Agez et al. (2020), potentially missing capital goods in PLCA value chains could not be estimated with IO, as the capital goods were not endogenized in the IO database used. The endogenization of capital goods in IO is seldom applied due to the lack of data on capital usage by industries. Nevertheless, taking advantage of a recent surge in its application at national and global scales (Chen et al., 2018; Miller et al., 2019; Södersten et al., 2018), we are now able to address the following research questions. *How can endogenization of capital goods be integrated in a streamlined hybridization framework? How do endogenized capital goods affect the results of THLCAs?*

1.3 The role and limitations of price data in hybrid LCA

PLCA process descriptions typically compile product requirements normalized per unit of the process's function, and this "functional unit" is typically in physical units. IO production functions also express product requirements per unit of the product or service supplied, but this functional flow is typically (though not always (Duchin, 1992; Merciai & Schmidt, 2017)) expressed in monetary units. In HLCA, the IO production function is therefore typically rescaled with price data, such that requirements are normalized proportionately to the same physical unit of functional flow as in the PLCA inventory.

This role of price data in HLCA leads to two issues. Firstly, if the price of the functional flow is not available (e.g., waste treatment processes in the ecoinvent3.5 database), the hybridization cannot be performed. Secondly, in the case of an PLCA process supplying a product whose price differs significantly from the average of the products of its sector, or in the case of highly aggregated sectors where prices are highly heterogeneous (see aggregation bias of IO (Asger Olsen, 2000; Morimoto, 1970)), the use of price data in the rescaling of IO production functions in HLCA becomes unreliable, leading to outliers (Agez et al., 2020; Yu & Wiedmann, 2018).

Relying on prices of functional flows to link IO and PLCA thus has serious limitations and initiatives to avoid the use of price data were developed (Dixit et al., 2015) albeit for specific categories of products. Relying on price data can especially prevent the hybridization when prices for these flows are unavailable or deemed unreliable. For example, in the tiered hybrid database of (Agez et al., 2020), nearly 1,000 processes of the ecoinvent3.5 database could not be hybridized due to price unavailability/unreliability. We will therefore address the question: *How can monetary and physical inventories be hybridized in a streamlined manner without relying on price data of the functional flow? Could such an alternative approach allow for the streamlined hybridization of the totality of a PLCA database, even including processes with products with uncertain prices?*

1.4 The limited coverage of environmental extensions of Multi Regional Input Output tables

Hybrid LCA consists in adding EEIO inputs to introduce requirements deemed missing in PLCA, i.e., complement the *technological* description of PLCA. The overarching goal of HLCA is to have a more complete estimation of elementary flows resulting from the production of a good or service. Yet, the amount of types of emissions covered by MRIOs is less than that of PLCA (e.g., 35 for EXIOBASE3 while ecoinvent3.5, a PLCA database, covers about 700). This is due to the priority national accounts have put on covering a given range of environmental stressors consistently across multiple sectors and to the difference in coverage of elementary flows of national accounts. MRIOs thus only select emissions covered by all countries. As a result, HLCA effectively completes emissions of main pollutants such as CO_2, CH_4, SO_2, etc. but is unable to complete more atypical emissions. For example, despite IO complement increasing the inputs of agricultural products taken into account in the value chain of manufactured goods, this increase led to no modification in the pesticide emissions in Agez et al. (2020). Due to this limited coverage, impacts assessed with MRIO databases are most likely underestimated, especially for impact categories involving a significant number of pollutants such as human toxicity or ecotoxicity (Arvesen et al., 2014). Therefore, the research question to be addressed: *How can the coverage of environmental extensions of MRIO tables be extended in a streamlined manner, such that these environmental extensions become commensurable with that of PLCA databases across all impact categories? What difference would this coverage increase introduce in HLCA database impacts?*

2. Aim and scope

This research aims to complete the remaining truncations of tiered hybrid LCA databases identified in the introduction through three corrective measures: (1) the integration of endogenized capital goods in the generation of a tiered hybrid inventory, (2) the hybridization of processes without a requirement for (unavailable or uncertain) price information and (3) an exploratory approach to estimate and integrate additional environmental extensions from a national IO table to an MRIO table. For these three measures, we studied their associated effects on 13 environmental impact categories using IMPACT World+ (Bulle et al., 2019). This research builds upon and extends the database hybridization framework developed in (Agez et al., 2020).

We will briefly introduce the methodology used in Agez et al. (2020). We will then describe how we introduced each new feature in the existing hybridization framework. The effects of these features will then be displayed and discussed. Throughout the article we will refer to the three measures as (1) capital add-on, (2) NFFBH (Non-Functional-Flow-Based Hybridization, see section3.3) and (3) emission add-on.

The research presented in this article was applied to two databases: ecoinvent3.5 and EXIOBASE3 (Ecoinvent centre, 2018; EXIOBASE Consortium, 2017; Stadler et al., 2018; Wernet et al., 2016) . The ecoinvent database was chosen for the transparency and large amount of processes covered. The EXIOBASE global MRIO database was chosen for high resolution and high types of emissions covered. The three measures introduced in this article were applied database-wide (and not to isolated processes) with a systematic, reproducible and transparent framework. The code to reproduce our work is available on Github (https://github.com/MaximeAgez/pylcaio) under an open-source license. Because our aim was to streamline the hybridization of thousands of processes following a set of generally applicable rules, the resulting hybrid database does not necessarily provide the best possible hybridization for each process.

3. Methods

In subsection 3.1, we provide a brief description of the tiered hybrid LCA method previously introduced by Agez et al. (2020). Then, we present three measures to cover gaps in the previously published method: the capital add-on (subsection 3.2), the NFFBH (subsection 3.3) and the emission add-on (subsection 3.4). Finally, we provide more detailed information about our case study (subsection 3.5).

3.1 Brief tiered hybrid LCA methodology

Tiered hybrid LCA, as applied in this article, consists in complementing data deemed missing from unit process inventories of PLCA using the data structure from IO to estimate these missing inputs. For example, the production of electric car includes no inputs of R&D services or computers, as the original compilation did not quantify these flows, and yet they may be estimated based on the use of services by the "Motor vehicles" sector in IO. It is a two-step process. First, *all* inputs of the corresponding sector from IO are added to the PLCA unit process inventory, using prices to convert the monetary dimension of IO to the physical dimension of PLCA. Some inputs are thus necessarily double counted. The second step is therefore to correct for this double counting, making sure that every input is only accounted once, either by PLCA or IO (Agez et al., 2019).

The streamlined hybridization of a given PLCA process is performed following equation (1):

$$c^{u}_{i,j} = \alpha(i,j,k) \times a^{io}_{i,k} \times \pi_j \tag{1}$$

where $c^{u}_{i,j}$ is the IO complement of sector i added to PLCA process j, $\alpha(i,j,k)$ is composed of different filters (of values 0 or 1) correcting for double counting incidents, $a^{io}_{i,k}$ is the IO coefficient from the technology matrix giving the purchase of products from sector i by sector k, with sector k being the sector to which process j belongs to and finally π_j is the price associated to the product of process j. For more information on this equation and all the variables, the interested reader is referred to Agez et al. (2020). Note that the understanding of everything underlying the factor $\alpha(i,j,k)$ is not required to comprehend the research presented in this article.

3.2 Endogenizing capital goods in tiered hybrid LCA

The endogenization of capital goods in IO results in a $\boldsymbol{K}$ matrix with the same dimensions as the technology matrix $\boldsymbol{A}$. The coefficient $k^{io}_{i,k}$ of the $\boldsymbol{K}$ matrix details how much capital good i was required this year, for the production of 1€ of products from sector k. Emissions due to capital formation are thus connected to the production of products in IO by adding $\boldsymbol{A}$ and $\boldsymbol{K}$. The traditional Leontief's equation with environmental extensions is thus modified as follows:

$$\boldsymbol{D} = \boldsymbol{C} \cdot \boldsymbol{S} \cdot \left(\boldsymbol{I} - (\boldsymbol{A} + \boldsymbol{K})\right)^{-1} \cdot \boldsymbol{Y} \tag{2}$$

where the $\boldsymbol{D}$ matrix gives all total impacts on the environment, the $\boldsymbol{C}$ matrix contains characterization factors, $\boldsymbol{S}$ contains environmental extensions, $\boldsymbol{I}$ is the identity matrix, $\boldsymbol{A}$ is the technology matrix, $\boldsymbol{K}$ is the capital matrix and $\boldsymbol{Y}$ is the final demand.

To integrate the endogenized capital goods inside the hybridization framework, equation (1) is modified as follows:

$$c^{u}_{i,j} = \alpha(i,j,k) \times \left(a^{io}_{i,k} + k^{io}_{i,k}\right) \times \pi_j \tag{3}$$

where $k^{io}_{i,k}$ is i-th row and k-th column element of $\boldsymbol{K}$.

In this research, we used the endogenized version of EXIOBASE3 developed by Södersten et al. (2020), as EXIOBASE was also the MRIO chosen by Agez et al. (2020) to produce their hybrid database. Södersten et al. (2020) applied the flow matrix method (Lenzen & Treloar, 2004) to the consumption of fixed capital, using WORLD-KLEMS (WORLD KLEMS Initiative, 2017), the EU KLEMS database (The Vienna Institute for

International Economic Studies, 2017) and national accounts to provide data describing capital goods transactions across products and industries.

Since capital inputs from IO are endogenized, they must not be double counted with those from PLCA. To follow with the methodology used in Agez et al. (2020), we relied on the STAM method (Agez et al., 2019) to correct for double counting. This method does not add IO inputs if a corresponding input is already accounted for by PLCA. In other words, when a capital good was already included in the unit process inventory of a PLCA process, the corresponding k coefficient for this capital good was not added to the unit process inventory, i.e., $\alpha(i, j, k) = 0$.

3.3 Non-functional-flow-based hybridization (NFFBH) to avoid price issues

EEIO analysis relies on so-called Leontief production functions, where the ratios between all the inputs and all the outputs are assumed to remain invariably fixed. For example, the ratio between iron ore, coal and labour inputs in the production of steel is assumed fixed, in a rigid "technological recipe". PLCA typically relies on similar fixed technology descriptions.

As previously discussed, in combining IO and PLCA production functions, the two must be rescaled to a common flow with price data. Traditionally, the common flow that defines this rescaling has always been the *functional flow*, expressed in physical units. The PLCA inputs are expressed per kg of steel output, while the IO requirements are rescaled with price data to express the inputs per kg of ferrous metal supplied, for example.

But if the ratio between *all* flows is fixed within each production function, then *any* flow that is thoroughly accounted for in both PLCA and EEIO production functions could theoretically serve as the common flow. In the hybridization of steel production, for example, we could very well rescale the EEIO production function such that its direct use of coal in physical unit equals that of the PLCA process description. Alternatively, if direct emissions of CO_2 are well accounted for in the two datasets, the EEIO description of ferrous metal production could technically be rescaled such that its direct CO_2 emissions equal that of the corresponding PLCA process. In both cases, the rescaled production functions could then be combined in a consistent hybrid analysis.

When should such non-functional-flow-based hybridization (NFFBH) be used? And if not the functional flow, which flow among all the input and output flows should be selected? Let us keep in mind that the objective of hybridization is to estimate as precisely as possible requirements that are missed in a PLCA process. Let us also keep in mind that EEIO production functions are the results of the aggregation of the "recipes" of multiple production activities within each sector; and that the more constant the ratio between two flows across these activities, the more confidently the scale of one flow can be used to estimate the other. In other words, when comparing multiple activities of a sector, the magnitudes of some flows will be well correlated with one another, while other flow pairs will not. Therefore, *ideally*, the combination of a PLCA and an EEIO production function should be based on the flow that, once converted to physical units, is best correlated to the EEIO flows that are missed in the PLCA description.

Unfortunately, the statistical distributions around EEIO coefficients and prices are almost never available. The practitioner must therefore fall back on heuristic to identify non-functional flows that are likely to be well correlated to all other inputs:

1. The flow must be thoroughly accounted for in both the PLCA and EEIO process descriptions. The NFFBH technique essentially assumes that this one flow is *not* truncated. This assumption may hold true for easily documented, environmentally important flows (fuel use, etc.)
2. For the flow to be well correlated to other flows and to serve as a good predictor of missing inputs, it should be of relatively high importance in the cost structure or the emission structure of the sector, technologically relevant, and expected to be displayed in similar proportions by all activities that constitute this sector.

For example, if we estimate that prices of products from the “Construction work” sector are highly heterogeneous (due to widely varying levels of value added across projects), then the supply flow of this sector (once converted to physical units) is most likely not an ideal candidate for estimating missing product inputs. We could turn, for example, to the flow of “Cement, lime and plaster”, which, being a staple of construction works with more narrowly defined prices, may be more closely correlated with the rest of the inputs. In other words, because of price heterogeneity, this example assumes that the calculated mass of cement used in production is a better predictor of the use of steel, electricity, services, etc. compared to the calculated physical amount of building. Missing inputs can therefore be estimated by reapplying the ratio “Cement, lime and plaster”/”missing inputs” using the PLCA quantity of “Portland cement”. Implicitly, it is assuming that the ratio “Cement, lime plaster”/”services” in IO is the same as the ratio “Portland cement”/”services” would be if PLCA covered services.

Mathematically, an estimated input $c^{u}_{i,j}$ would thus be determined relying on equation (4) instead of equation (3):

$$c^{u}_{i,j} = \alpha(i,j,k) \times (a^{io}_{i,k} + k^{io}_{i,k}) \times \frac{a^{lca}_{m,j} \times \pi_m}{a^{io}_{n,k}} \quad (4)$$

where $a^{lca}_{m,j}$ is the quantity of flow m (used as the common flow to rescale other inputs with) required for the production of j according to a selected PLCA database, $a^{io}_{n,k}$ is the quantity required of products from sector n $(m \in n)$ for the production of the sector k in which is included process j and π_m is the price of flow m.

Following up on the previous example to make it clearer: the determination of the amount of IO complement “services” (i) in the hybridization of PLCA process “passive house construction” (j) with the “Construction work” sector (k) is based on the amount of PLCA process “Portland cement” (m) used by the “passive house construction” and the amount of “Cement, lime and plaster” (n) used by the “Construction work” sector. Instead of relying on the price of the “passive house construction” (π_j), the hybridization thus relies on the price of “Portland cement” (π_m) to estimate how much “services” the production of the “passive house construction” required.

The same logic can be applied using elementary flows. For example, the service inputs of a “waste treatment landfill” process can be determined using the amount of direct emissions of CO_2, because in this case, the direct emissions of CO_2 probably have a better correlation with other inputs. The estimation of missing input $c^{u}_{i,j}$ would therefore follow equation (5):

$$c_{i,j}^{u} = \alpha(i,j,k) \times (a_{i,k}^{io} + k_{i,k}^{io}) \times \frac{s_{m,j}^{lca}}{s_{n,k}^{io}} \tag{5}$$

where $s_{m,j}^{lca}$ is the amount of elementary flow m used by process j and $s_{n,k}^{io}$ is the amount of elementary flow n used by sector k.

Note that there is no more dependency to prices in equation (5), as elementary flows are compiled in physical units in both PLCA and IO databases. The amount of "services" is estimated based on the ratio of direct emissions of, e.g., "PLCA CO_2" (m) on direct emissions of "IO CO_2" (n), assuming again, that the ratio "CO_2/services" would be identical between IO and PLCA, if PLCA covered services. The complete list of common flow/sector combinations used in this study can be found in SI2.

3.4 Estimating environmental extensions from national to global MRIOs

Currently, the coverage of different types of elementary flows across all existing environmentally extended MRIOs is highly incomplete. To fill this gap, we need to estimate missing environmental extensions across all sectors and regions based on other (less geographically exhaustive) data sources. PLCA databases were briefly considered as a potential data source, but they do not match the technological coverage of MRIOs. Instead, this article explores the use of environmental extensions of national EEIOs to estimate elementary flows for all regions of an MRIO. In other words, the sectors of selected countries with detailed elementary flow accounts are used as "geographical proxies" for similar sectors in other regions with less exhaustive statistics on exchanges with the environment. A parallel can be drawn with the use of geographical proxies in the pedigree approach of PLCA (Ciroth et al., 2016; Muller et al., 2016).

The expanded satellite matrix of the MRIO table $\boldsymbol{S'}$ is then linked to an expanded $\boldsymbol{C'}$ matching the added environmental extensions to corresponding characterization factors. Both matrices are then introduced in equation (2) as follows:

$$\boldsymbol{D} = \boldsymbol{C'} \cdot \boldsymbol{S'} \cdot \left(\boldsymbol{I} - (\boldsymbol{A} + \boldsymbol{K})\right)^{-1} \cdot \boldsymbol{Y} \tag{6}$$

In this study, as a first demonstration, we completed the environmental extensions from EXIOBASE3 adapting the methodology of (Muller, 2019) and using environmental extensions from USEEIO (Yang et al., 2017a), a national EEIO for the United States. USEEIO was chosen for its comparable list of stressors to PLCA databases (several hundreds of elementary flows), its relative recency (2012) and its open-source license. In choosing USEEIO, we had to deal with two aggregation issues, i.e., at the technological level and at the extensions level. Concordances between EXIOBASE and USEEIO therefore had to be produced to match both sectors and extensions. Only missing emissions to EXIOBASE (e.g., acrolein released in the air) were added and existing emissions were not modified (e.g., CO_2). In cases where categories of pollutants were present in both databases (e.g., NMVOCs), but additional emissions from the same family were explicitly reported in USEEIO (e.g., formaldehyde), we added these additional emissions to EXIOBASE's extensions. Otherwise, if a category of pollutant is only present in EXIOBASE (e.g., HFC) but that USEEIO describes each pollutant of this family specifically (e.g., HFC-116), specific pollutants were not added as they were considered to be already included into the category of EXIOBASE. Adding them would result in double counting.

3.5 Case study

In this article, we completed the ecoinvent3.5 cut-off version (Ecoinvent centre, 2018) with the product x product EXIOBASE3.7 matrix, base year 2011 (EXIOBASE Consortium, 2017). The technology matrix of EXIOBASE was compiled using an industry-technology construct. The capital add-on was applied using the product-by-product capital matrix base year 2011 (Södersten, 2020) . We used USEEIOv1.1 for the emission add-on (Yang et al., 2017b). Finally, we used the midpoint v1.28, global default values from IW+ (Patouillard, 2019). For simplicity, we use abbreviated names for the impact category of IW+ in our presentation of results (see SI1 for concordance with actual IW+ nomination and units of impact categories).

Three impact categories of IW+ were excluded from this study. The impact on ionizing radiations could not be studied as neither EXIOBASE nor USEEIO track pollutants of this impact category. The land transformation impact category was excluded as EEIO does not keep track of the original state of the land used. Finally, ozone layer depletion was excluded as results obtained for this impact category were not deemed robust enough (refer to SI1 for more details).

4. Results

This result section investigates the effects of implementing the three measures presented in this article on the environmental impact results. First, we explore the effects of expanding the environmental extensions of an MRIO on the global economy impact scores. Second, we hybridize a PLCA database with an MRIO database accounting for all three additional measures and investigate their effects when compared to impact scores of the non-completed version of the PLCA database. Finally, we present the sources for data, results and codes generated to compute the case studies.

4.1 Expanded environmental extensions of EXIOBASE

Originally, EXIOBASE3 included 32 different emissions to the air, 2 emissions to water and 1 emission to soil for a total of 35 emissions. After estimation of additional environmental extensions, EXIOBASE environmental extensions included 832 emissions to the air, 832 emissions to water and 137 emissions to soil, for a total of 1766 added emissions. Other environmental extensions from EXIOBASE were left untouched (i.e., mineral resources, water flows and land use) as they were as complete as extensions from USEEIO.

The characterization of these additional 1766 elementary flows affected the impact scores of 9 impact categories of IW+ across all sectors from EXIOBASE. Figure 1 shows the relative increase (in percent) of the impact of the global economy (in 2011), between the original version of EXIOBASE3 and the expanded version.

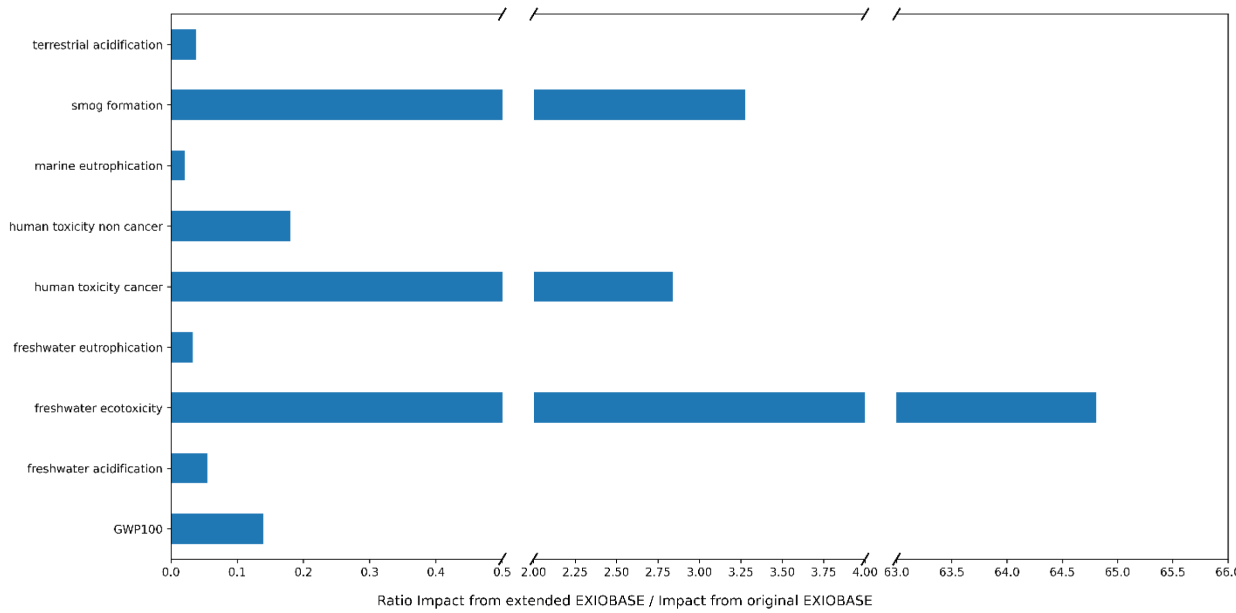

Figure 1: Percentage increase for the total impact scores of the world economy (calculated with EXIOBASE3 2011) after estimation of additional environmental extensions based on USEEIO for affected impact categories of IW+. Note that the x-axis was made discontinuous to allow the visualization of all impact categories. Most impact categories are unaffected or marginally affected by the additional environmental extensions. The total footprint for freshwater ecotoxicity however, is increased by nearly 65%, indicating that EXIOBASE in its original state is not adapted to enable the study of ecotoxicity impacts.

We can distinguish three groups of impact categories. The first group is composed of impact categories for which the increase is lower than 0.2%, namely, terrestrial acidification, marine eutrophication, human toxicity non cancer, freshwater eutrophication, freshwater acidification and global warming potential. Given the limited effect of the additional environmental extensions on these impact categories, we can conclude that EXIOBASE's 35 original emissions, were already covering the most relevant elementary flows. For smog formation and human toxicity cancer, the increase in both impact scores of EXIOBASE is around 3%, mainly due to toluene flows for smog formation and to formaldehyde flows for human toxicity cancer. Finally, the impact score for freshwater ecotoxicity increases by 65%, mainly due to aluminum emissions and various pesticides elementary flows. EXIOBASE in its original state is therefore not adapted to study this impact category. The interested reader can find which emissions were added, classified by impact categories in SI2.

4.2 Effect of the measures on PLCA impact scores

The corrective measures of this article have different effects. The capital and emission add-ons increase the impact score of each process of the database by a given amount, leading to an overall increase of all impact scores. The application of the NFFBH, in contrast, allows some processes that had previously been excluded in Agez et al. (2020) to now be hybridized. As such, it does not alter the impact score of all processes of ecoinvent, unlike the two other measures.

The effects of the capital and emission add-ons were represented as the relative median impact score increase stemming from the IO inputs added to each unit process inventory, for 13 midpoint impact categories of IW+ (Figure 2). In other words, the median of impact score represents the increase when compared to the *original* version of ecoinvent3.5. The blue part of the pie charts represents the increase due to streamlined hybridization relying solely on product flows (following equation 1), as applied in Agez et al. (2020). It puts in perspective the effect of the new measures compared to what was previously achieved. The green part represents the effect of the capital add-on and the red part displays the effect of the emission add-on. Furthermore, we separated the different processes of ecoinvent into 12 categories of products to avoid biases due to the coverage of ecoinvent, i.e., nearly 40% of processes in ecoinvent model electricity generation technologies and markets. The number of processes included in each category is displayed under the name of the category. The application of NFFBH allowed to hybridize 982 more processes. The distribution of these processes is indicated with the nffbh acronym. Note that only 6,082 processes are hybridized, while ecoinvent3.5 includes 16,022, because market and internal processes should not be hybridized to avoid double counting as discussed in Agez et al. (2020).

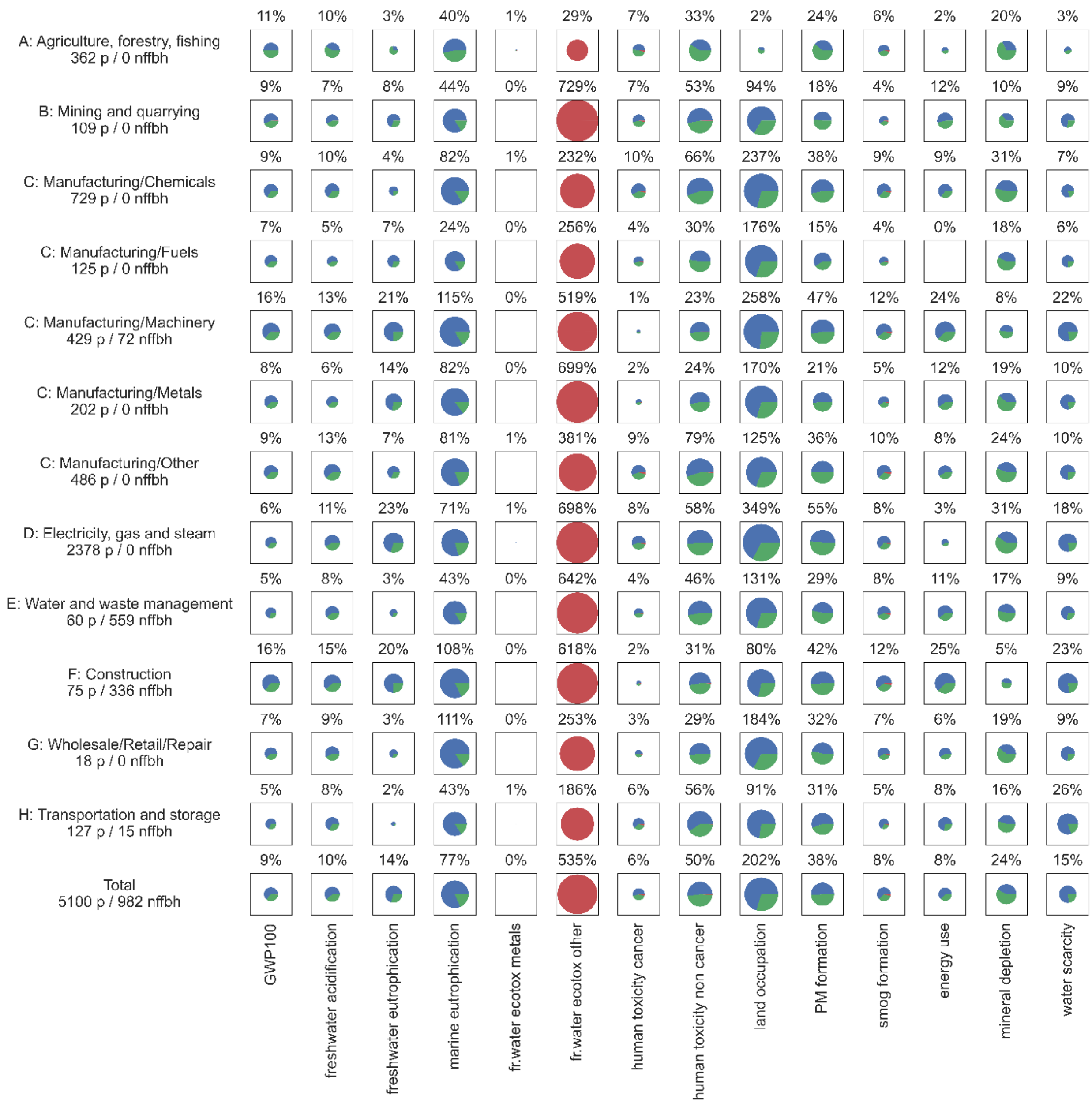

Figure 2: Median percentages of impact score increase after hybridization for 13 midpoint categories of IW+ (freshwater ecotoxicity with divided in 2 sub-categories) for 12 categories of products. The distribution of the 6082 hybridized processes of ecoinvent across the 12 categories of products is shown under the name of the category. Processes hybridized using the NFFBH are tagged with the nffbh acronym. The median of impact score increase is represented by the size of each pie chart (in logarithmic scale). The blue part of each pie chart represents the increase due to the hybridization as presented in Agez et al. (2020)*. The green part represents the increase brought by the capital add-on. Finally, the red part represents the effect of the emission add-on. The application of NFFBH allowed to hybridize 982 more processes, mainly waste treatment processes and buildings which are found in the E and F product categories. Data to reproduce this graph is available in SI3.*

Among the 13 midpoint impact categories of IW+ that could be linked to EXIOBASE and its newly estimated extensions, 10 display median increases ranging from 6% to 50% which matches with the expected range of increase due to hybridization found in (Agez et al., 2020) and (Yu & Wiedmann, 2018), though these articles did not cover as many impact categories. We will further explore the remaining 3 categories.

The category which increases the most due to hybridization is land occupation, with a median total increase of 202%. The disaggregation per category of products shows that agriculture and forestry are only marginally affected for this impact, in contrast with the lifecycle of products from other categories. A major impacting input is therefore missing from value chains of non agriculture/forestry related processes. We know that ecoinvent (and PLCA in general) struggles when it comes to introducing services and other seemingly unrelated inputs. One of the services that most companies require and that impacts the land occupation category is the “hotel and restaurant service”. Because of the arable lands that are cultivated to provide the food for this service, the land occupation indicator significantly increases after hybridization.

The marine eutrophication impact also rises considerably (89%). Major pollutants for this category (nitrogen emissions to water and ammonia emissions to air) come from agriculture and textile activities. Once again, the absence of restauration services in ecoinvent could thus explain this important increase. Similarly, uniforms provided by companies to their employees could also contribute.

The freshwater ecotoxicity category was separated in two sub-categories (one accounting for metal emissions only and the other accounting for all other substances) because metals pose a particular challenge in terms of their coverage in each database as well as the high magnitude and uncertainty of their impacts. Impacts due to metal emissions are only marginally increased by the hybridization while the impacts due to other pollutants (e.g., pesticides, aromatic compounds) are significantly influenced by hybridization.

For PLCA practitioners specifically, Figure 2 displays the relative importance to perform hybridization with (or without) the measures proposed in this article, and thus should help prioritizing efforts in using hybridization with or without these measures. If the land occupation impact of the production of potatoes is being studied, the hybridization should only have a marginal impact on the results. If the land occupation of the production of coal electricity is studied however, not hybridizing should result in a significant under-estimation of the impact.

Throughout this section we chose to operate with median increases only, as they are more representative than the average increases. That is because the average is heavily influenced by outlier values. In our case study, across each impact category we have several points reaching thousands level of increase which unjustifiably inflate average values. The streamlined hybridization framework presented in this article obviously fails for these processes. However, as was pointed out in the aim and scope section, our goal is not to perfectly hybridize all processes of ecoinvent, rather, our goal is to hybridize thousands of processes in a streamlined fashion. Figure 3 represents the distribution of values for the increase across all ecoinvent processes through violin plots in logarithmic scale. Average values are represented by black crosses, median values by black dots, 1st and 3rd quartiles by black bars. We can see that average values are regularly greater than 3rd quartiles.

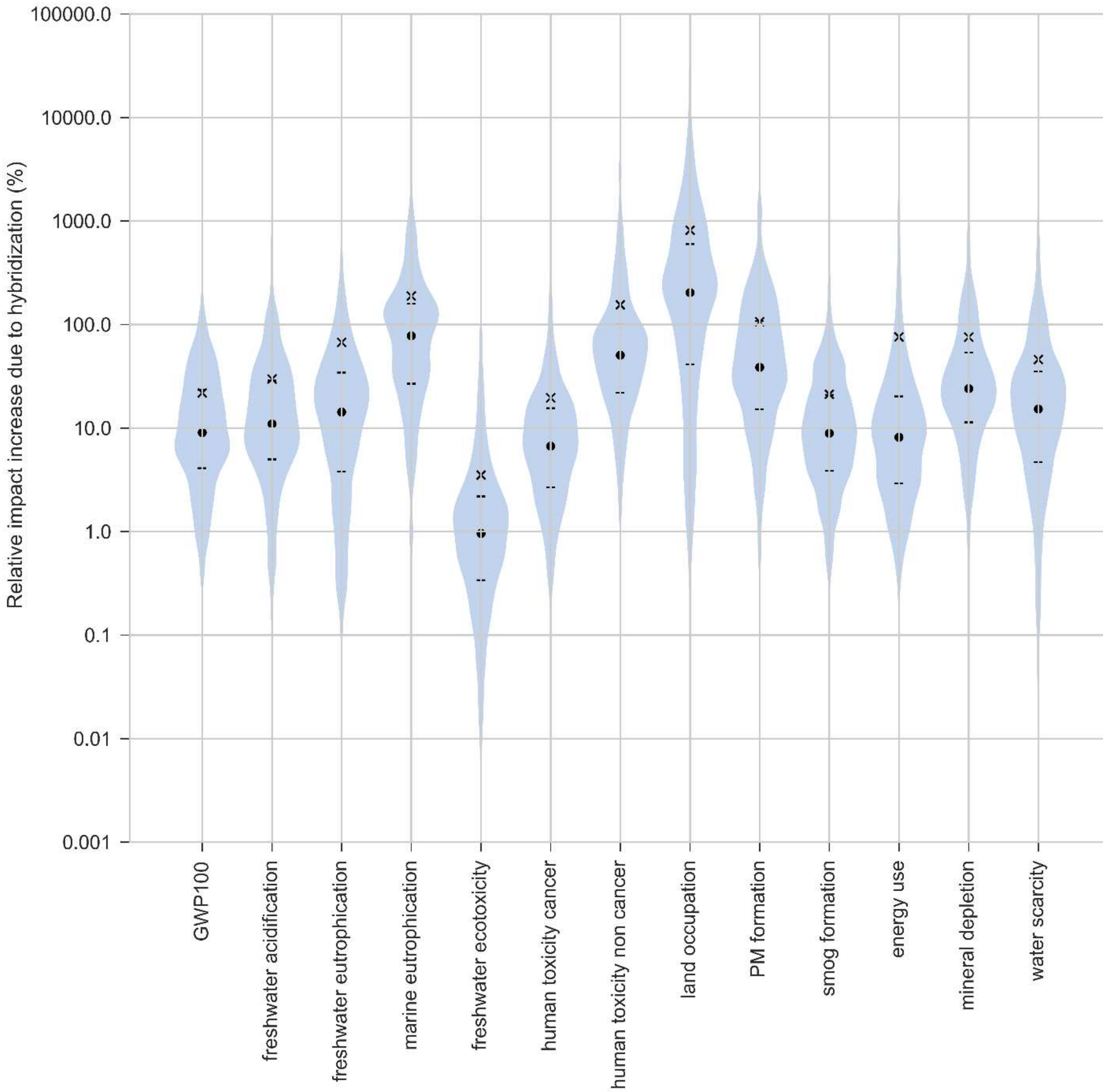

Figure 3: Violin plots in logarithmic scale representing the distribution of impact score increase values for all ecoinvent processes. Medians are represented as black dots, means as black crosses, 1st and 3rd quartiles as black bars

4.3 Datasets produced in this study

This study resulted in the creation of four datasets: (1) the upstream cut-off matrix $\boldsymbol{C^u}$ as calculated by equation 6, which contains all estimated missing inputs (e.g., services) for each process of ecoinvent3.5 (http://doi.org/10.5281/zenodo.3890379), (2) a characterization matrix linking the environmental extensions of EXIOBASE3 to the IW+ impact assessment method (http://doi.org/10.5281/zenodo.3955079), (3) the expanded environmental extension matrix of EXIOBASE3 (estimated using USEEIO's environmental extensions) and a characterization matrix linking the added flows to IW+ (http://doi.org/10.5281/zenodo.3890321), (4) a characterization matrix linking ecoinvent3.5 elementary flows to IW+ characterization factors (http://doi.org/10.5281/zenodo.3890367).

The code for completing ecoinvent3.5 with EXIOBASE3 relies on pylcaio v2.0 (https://github.com/MaximeAgez/pylcaio). To use pylcaio v2.0, access to ecoinvent3.5 and EXIOBASE3 databases is required. The software is under a GNL open-source license. It can thus freely be copied, modified and re-used under the same license. The software does not include a user-interface. As of pylcaio v2.1, generated hybrid databases can be exported to brightway2 (https://brightway.dev) and can thus be read on their latest graphical user interface (Steubing et al., 2020).

5. Discussion

5.1 Limitations of estimating environmental extensions from USEEIO to EXIOBASE

In the result section, it was shown that the estimated environmental extensions were paramount to the study of the freshwater ecotoxicity impact indicator while using EXIOBASE. It also appears that a non negligible quantity of smog formation and human toxicity cancer impacts is missed without the estimated environmental extensions. A better coverage of environmental extensions should thus be prioritized by MRIO databases. The methodology presented in this article however, has some overbearing limitations. By re-applying US emission factors to other countries, it is assumed that technologies from other countries have the same performance than in the US. Moreover, regulations also play a disruptive role in this estimation. Some products (e.g., pesticides) used in the US are banned in other countries and vice versa. By simply applying US emission factors to these countries, it is assuming the same products are used in the world.

Some improvements to the methodology could thus be performed. For instance, a reference country per continent, based on a few well-developed national IO tables, could be used to get a better estimation, e.g., estimate Vietnamese emissions based on China's national EEIO. Another lead could be to rely on national emissions databases to identify sectors in countries that tend to pollute more (or less) than US sectors and apply a multiplicative factor to the estimated extensions.

5.2 Limitations inherent to the methodology in Agez et al. (2020)

Even though this article strived to correct some of the limitations of Agez et al. (2020) through the addition of the three measures introduced, this research still inherits some of the limitations of the previous article: (1) this work relies heavily on matching products or elementary flows between different databases and is therefore prone to errors; (2) the prices used came from ecoinvent and were compiled pre-allocation while we hybridized the ecoinvent cut-off version, prices might therefore not be adapted; (3) as in any hybrid analysis, the aggregation bias of IO leads to uncertainties which are not quantified in this project; (4) the effect of the variability of prices on the results is not evaluated. Note however, that there is a linear relationship between the IO complement and the price. If the price used for hybridization is overestimated by 20%, the IO complement itself would be overestimated by 20% as well.; (5) the impact of the choice of the MRIO database used on the results is not quantified; (6) the influence of the method to correct double counting is not assessed, but preliminary work on the issue already exists (Agez et al., 2019).

5.3 The case of ecotoxicity

As shown in Figure 2, the hybridization does not influence the freshwater ecotoxicity in the same fashion when looking at metal emissions or other emissions. Indeed, inherently, both ecoinvent and EXIOBASE/USEEIO do not put the same focus on these pollutants. We compared the share of metal/other pollutants, scaled up to the whole economy (results in SI2). Obviously, ecoinvent does not cover the whole economy, nevertheless, the distribution of the covered pollutants should stay representative. 99.99% of the ecotoxicity impact of ecoinvent stemmed from metal emissions. The combined EXIOBASE/USEEIO database, on the other hand, calculated that only 33% of the total impact was caused by metal emissions. Since both impacts were assessed using the same impact method, biases from characterization method should be minimal. There is therefore an inconsistency in the treatment of ecotoxicity between ecoinvent and EXIOBASE/USEEIO. In other words, either ecoinvent covers metals significantly better than other pollutants or EXIOBASE and USEEIO significantly underestimate the amount of metal emissions. The latter can be an inherent product of IO methodology however. Since IO tables are focused on annual data, they do not include long-term emissions and most likely only cover "instantaneous" metal emissions. The coverage of ecotoxic pollutants is therefore an area of improvement for data collection in both PLCA and EEIO databases.

5.4 Improving capital inputs in PLCA

In this study, STAM was used to correct for double counting to keep the methodology previously used in Agez et al. (2020). One of the core assumptions of STAM however, is that if a product is already covered by the PLCA database, the data will not be complemented by IO inputs. In other words, if a capital input is already provided by ecoinvent, it was not complemented with EXIOBASE capital inputs. The endogenized version of EXIOBASE however, provides a more detailed coverage of capital inputs. The PLCA community could therefore extrapolate these capital inputs to improve the capital goods coverage in PLCA. To enable the extrapolation, an average capital formation and consumption over a period (using EXIOBASE time series for example) would be needed. This could result in better estimates of capital inputs in PLCA databases.

5.5 Regionalization of impacts in EXIOBASE

This project allowed the linkage of the different datasets used to IW+. This impact method enables the regionalization of impacts. For specific impact category, a pollutant emitted in Australia could impact more (or less) than the same emission in China. One of the struggles of using regionalized characterization factors is that the inventory must be spatialized, i.e., a location must be attributed to the emission that takes place (Patouillard et al., 2018). In PLCA, most of the time, the location of the emission is not precise, as many processes are defined for broad regions (e.g., Europe) or as global processes. For MRIOs on the other hand, such spatialization could mostly be done at the national level, as emissions are given for each sector in each country. The use of regionalized characterization factors would thus be interesting in IO to increase the accuracy of impact scores.

6. Conclusion

This article built on the previously developed method of Agez et al. (2020) by introducing three corrective measures: the endogenization of capital goods and their integration into the hybridization framework, the hybridization of processes with unreliable/unavailable prices and the estimations of additional environmental extensions. These three measures further increased the estimated truncation level of PLCA previously found in Agez et al. (2020). This study looked at 13 impact categories, using the IMPACT World+

impact method, instead of the 4 categories used previously. It allowed us to see that hybridization is paramount when looking at particular impact categories, e.g., the land occupation impact category saw a 202% median increase across all ecoinvent processes. This study thus helped practitioners determine when hybridization should be prioritized and if including the measures of this article is relevant. Even if the method used in this study to estimate new environmental extensions for EXIOBASE is limited, the results still showed that EXIOBASE is currently not equipped to study the freshwater ecotoxicity impact categories.

The PLCA and IO communities have mostly walked their own path when it comes to system description and database compilation. Hybrid LCA and this article try to bring these two communities together in using the strength and shortening the weakness of one another. Potential leads identified during this research are the improvement of capital representation in PLCA based on capital representation in IO, the implementation in IO of regionalization characterization factors used in PLCA and the need for both communities to enhance the coverage and characterization of ecotoxicity pollutants. PLCA and MRIO database compilation teams would thus greatly benefit from working together.

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