Deriving material composition of products using life cycle inventory databases

Amatuni, L.T.; Steubing, B.R.P.; Heijungs, R.; Yamamoto, T.M.; Mogollón J.M.

DOI: 10.1111/jiec.13538

METHODS ARTICLE

JOURNAL OF INDUSTRIAL ECOLOGY WILEY

Deriving material composition of products using life cycle inventory databases

Levon Amatuni | Bernhard Steubing | Reinout Heijungs | Tales Yamamoto | José M. Mogollón

Institute of Environmental Sciences (CML), Leiden University, Leiden, The Netherlands

Correspondence
Levon Amatuni, Leiden University, Haverstraat 51, Leiden 2311NN, Netherlands.
Email: l.t.amatuni@cml.leidenuniv.nl

Editor Managing Review: Wei-Qiang Chen

Funding information
H2020 European Institute of Innovation and Technology

Abstract

Understanding the detailed material composition of the various industrial and consumer products is essential for implementing efficient recycling practices and policies, conducting material flow analyses, and facilitating a transition toward a circular economy. However, existing data sources are limited in their product and material coverage. Currently, no source or methodology allows such data to be obtained in a relatively uniform, updated, and accessible manner across a diverse range of products. This work presents an approach that allows estimating the material composition of thousands of products using available life cycle inventory (LCI) databases. Methodologically, this is implemented by splitting the physical flows that describe supply chains in LCI databases into "incorporated" and "not incorporated" fractions using an incorporation parameter. Building primarily on existing matrix-based life cycle assessment calculations, this approach can be used to calculate the material content of products. A generally applicable mathematical model, as well as a ready-to-use software, is presented for future practitioners. To demonstrate the robustness of the proposed method, a case study involving three metals and plastic in three consumer goods has been conducted based on the ecoinvent database. Our method delivered accurate material content estimates (i.e., weight fractions of materials in products) with an average relative error of 26% and an absolute error of 1.1% (between our estimates and existing values).

KEYWORDS
industrial ecology, LCI database, life cycle assessment, material composition, material footprint, product composition

1 | INTRODUCTION

The transition toward a more sustainable society requires a thorough understanding of the material economy, including the composition of the goods manufactured and consumed by the society. In particular, it has been advised previously that product composition information supports practitioners of material flow analysis and life cycle assessment (LCA) while facilitating the implementation of efficient recycling practices, policies, and the circular economy (Hoekstra & van den Bergh, 2006; Horta Arduin et al., 2020; Jensen & Remmen, 2017).

Due to rapid technological innovation and miniaturization, product complexity has increased significantly (Singh & Ordoñez, 2016). Manufactured goods require a greater variety of materials than ever before. Likewise, materials are present in increasingly smaller quantities, complicating composition assessments and material recycling (Stigson et al., 2006; Teehan & Kandlikar, 2013).

Unfortunately, due to highly complex supply chains, intellectual property-related protections, and market competitiveness, manufacturers are usually either incapable or reluctant to disclose their products' comprehensive and detailed material content. Although some governments have started to acknowledge the importance of the mandatory environmental product declaration (EPD) by industries (Passer et al., 2015), currently, so-called bills of materials in the existing EPDs are quite limited.

Different approaches have been implemented in the past to obtain and store information on the material composition (MC) of products. While various laboratory-based materials analysis techniques offer accurate information, they are expensive and time-intensive. Based on reports from such physical tests and manual surveys, numerous narrowly specialized studies are conducted, usually on the presence of a specific set of substances in specific applications. As an example, Oguchi and colleagues (2011) have compiled information on the content of several metals in different consumer electronics. At the same time, several larger-scale ad hoc databases became available. For instance, publicly disclosed material safety data sheets were used to collect quantitative and qualitative data on chemicals in consumer products, primarily cosmetics and chemical products (Dionisio et al., 2018). Another material intensity database has been recently developed and customized for buildings (Heeren & Fishman, 2019).

These approaches, however, encompass the following challenges. First, the product MC data are highly dispersed in multiple sources and formats. Second, most of the time, the related data sources cover only specific product groups and materials, for example, chemicals in cosmetics (Dionisio et al., 2018) and silver in tube rays (Oguchi et al., 2011). As a result, the existing MC data harvesting methods are rather time-consuming and limited. Finally, product designs and technologies and their MCs are changing rapidly, and existing data sources are becoming outdated quickly and difficult to update. In this study, we demonstrate that utilizing life cycle inventory (LCI) databases can help overcome such challenges.

LCA is a widely applied method to assess the environmental footprint of products and services and relies on LCI databases, which contain thousands of detailed technical descriptions of human activities, so-called *unit processes*, and their interactions with the environment (ISO, 2006). The flows described in LCI databases include thousands of material flows related to the delivery of thousands of products.

Several studies have previously explored the concept of material intensity (as of the total material burden along the supply chain) within the LCA framework (Lettenmeier et al., 2009), and the LCI databases have been previously used to estimate the material footprint (MF) of goods and services (Saurat & Ritthoff, 2013; Wäger et al., 2015; Wiesen et al., 2014; Williams et al., 2002). It has also been suggested by Wiesen et al. (2014) to account for the unused extraction-related resources along the supply chains in the ecoinvent database to estimate the total material impact per service more accurately. Other studies reviewed how the material dissipation concept (i.e., flows to inaccessible sinks or stocks) is positioned within the LCA framework (Beylot et al., 2020; Zimmermann & Gößling-Reisemann, 2013). None of these studies, however, researched how the MC of products can be estimated.

Currently, there is no source and methodology in place that allows such MC data to be obtained in a relatively uniform, updated, and accessible manner for a broad range of products and materials. To respond to such a need, we:

(i) present a uniform approach to estimate detailed product MCs based on existing LCI databases by distinguishing between resources that are incorporated versus those that are not incorporated into products over their life cycle; within the existing unit process data (e.g., laptop manufacturing), various raw material inputs (e.g., copper) are mixed with other physical components (e.g., laptop's display) and auxiliary inputs (e.g., factory);

(ii) demonstrate the implications and the accuracy of the proposed methodology in practice for three consumer products while providing open-source software for practitioners (Amatuni, 2023);

(iii) propose a conceptually new technical improvement of such LCI databases that would allow this approach to become much more reliable and widely applicable in the future, as existing LCI databases conceal potentially valuable composition information that is often available at the time of their compilation.

To our knowledge, this is the first attempt to filter out auxiliary inputs from the unit processes to obtain the MC of products on a system level within the LCA framework. At the same time, a similar idea could be observed in the waste input–output analysis proposed by Nakamura and Nakajima (2005), Nakamura et al. (2011), and Ohno et al. (2018). There, within the input–output analysis (IOA) framework, it has been proposed to depict the material flows in the economy filtering out such auxiliary inputs from the industries. To acknowledge the original contributions of these studies, we adopt the existing terms wherever possible.

The paper first introduces the key concepts to our newly proposed methodology. In particular, different categories of material flow within the LCI framework are defined, classified, and visualized. Second, the mathematical model to estimate the MC of products within the computational structure of LCA is presented and exemplified. Then, the application of such an MC estimation method is tested for a diverse set of consumer goods (laptops, passenger cars, and refrigerators) and materials (copper, aluminum, tantalum, and plastic) in the ecoinvent database, showing its robustness. Finally, the results and limitations of the proposed methodology, along with the suggestions for the future development of LCI databases, are discussed.

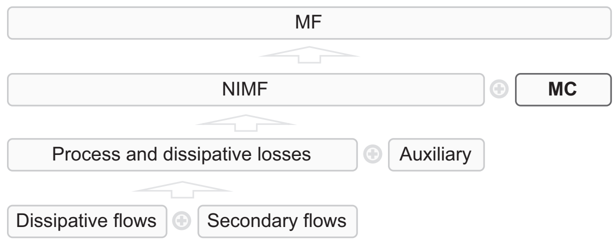

FIGURE 1 Material flows hierarchy defined in the paper. MF, material footprint; MC, material composition; NIMF, non-incorporated material footprint.

2 | MATERIAL AND METHODS

2.1 | Material flow classification

In this study, *material* is used as an umbrella term for the elements, constituents, or substances that comprise (or are used to make) a product or commodity (Webster, 2022). We discern between natural (e.g., copper, wood) and synthetic (e.g., plastic, glass) materials. While natural materials are extracted, refined, and processed along the supply chain, they do preserve their elemental and valuable substance in their initial natural form. Synthetic materials, on the other hand, are made chemically and are only obtained along human production chains. Additionally, materials could be either elemental (e.g., copper) or more complex (e.g., metals in general).

Here, product MC is defined as the content of a specific material in a tangible product. This is distinguished from the MF of a product that describes the cumulated input of that material along the supply chain "from the cradle to the point of sale" (Lettenmeier et al., 2009). The MF is also sometimes referred to as material input per service or MIPS (Schmidt-Bleek, 1994), and the product material footprint or PMF (Mostert & Bringezu, 2019), even though these terms could imply different life-cycle boundaries and application methods. They should not be confused with similar terms for the national-level footprint assessment (UNEP, 2021; Wiedmann et al., 2015). In this study, we consider the MF of a product (compared to a service) that includes its cradle-to-product life stages only, even though cradle-to-grave boundaries for the MF could be considered instead. For any given material of interest, the MC of a product is always lower or equal to its MF, as the latter value covers all the extracted material needed for a unit of production. The MF includes both the *incorporated* (e.g., plastic content in a laptop) and the *non-incorporated* (e.g., plastics tables in the factory that manufactures that laptop) material footprint (NIMF) of a product. At the same time, the MC describes the material incorporated (into the final product) only. Accordingly, MF = MC + NIMF.

The incorporated material flows, such as the physical components or the required materials, are entirely contained within the corresponding products. In contrast, the non-incorporated material flows, such as the *auxiliary* flows or *losses*, do not become part of the manufactured product. The *auxiliary flows* are the capital and other goods used during production that are not intended to become part of the product (e.g., copper in machinery used for producing a laptop). The losses are either the *secondary flows*, which are the so-called process losses that have a residual value and re-enter the supply chain (e.g., copper scraps related to the production of a laptop), or the *dissipative flows*, which are inaccessible losses such as emissions to the environment (Beylot et al., 2020). A diagram depicting the introduced flows hierarchy is presented in Figure 1.

2.2 | Material incorporation

LCI databases are organized collections of unit processes (i.e., LCI datasets) that describe human activities (e.g., manufacturing a laptop) and their related exchanges with the environment and the product systems (Ciroth & Burhan, 2021). Here, we define a *reference product* as a process' main functional output (if it exists). Additionally, we assume that each unit process has only one reference product (e.g., a laptop).

The LCA methodology distinguishes between two types of flows or exchanges (ISO, 2006):

- *Elementary flows* describe the interaction of human activities and the environment (e.g., the extraction or *input* of copper ore from the environment into the refinement process; the release or *output* of carbon dioxide into the atmosphere);
- *Intermediate or product flows* describe the exchanges between human activities (e.g., refined copper input to vehicle manufacturing; waste outputs by the factory to be treated by recycling activity).

To be able to use LCI databases to assess the MC of a product, information needs to be available on the extent to which every process input is materially incorporated into the reference product of the corresponding unit process. This has to be known over the life cycle (i.e., supply chain) of

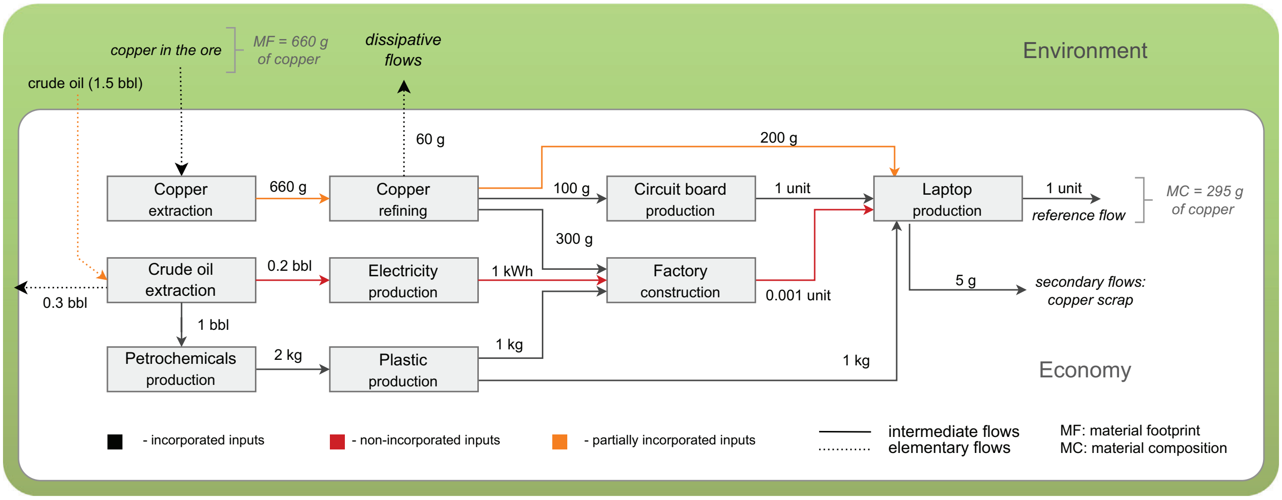

FIGURE 2 Simplified supply chain for a single laptop manufacturing in terms of the corresponding copper and plastic use. Distinguishes elementary and intermediate flows as well as the levels of incorporation for the inputs along the chain. MF, material footprint; MC, material composition; bbl, one barrel. Underlying data are available in a matrix format in Sheet5 of Supporting Sheets.

the product of interest (e.g., plastic is fully incorporated into plastic packaging in the production process of plastic packaging; the plastic packaging, in turn, is not at all incorporated into the laptop at a later stage of the laptop production).

Thus, to serve the purpose of this study, each existing elementary and intermediate flow in a chosen LCI database needs to be characterized by an additional parameter. The value of this parameter can be either 1 (meaning fully incorporated), 0 (meaning fully non-incorporated), or any value between 0 and 1 (meaning partially incorporated). Partially incorporated inputs are those that carry both incorporated and non-incorporated material flows at the same time (e.g., refined copper input that goes through partial process losses of 2.5% during laptop manufacturing).

Figure 2 exemplifies the distinctions mentioned above (MF and MC, elementary and intermediate, and incorporated and non-incorporated material flows and process inputs) and aligns them with the general LCI framework for a simplified laptop manufacturing supply chain, allowing estimation of the copper content in a laptop.

If we trace the upstream supply chain of the reference product of interest, it is possible to trace the material flows required to deliver that final product, the MF. In particular, it can be seen that such laptop production requires 200 g of copper as direct input plus 100 g of copper in the circuit board as well as 0.001 factories to manufacture one laptop (assuming for simplicity that one factory produces 1000 laptops), which in turn needs 300 g of copper (per one laptop output) for its construction. As a result, the MF of the laptop is 660 g of extracted copper metal, and 10% of it is lost during refining. At the same time, it can be seen that only 295 g of that copper is incorporated in its body (the MC) when only the incorporated flows are considered (the factory requiring 300 g omitted) and the two partially incorporated inputs are corrected for dissipative (60 g) and manufacturing process (5 g) losses.

In practice, such economic supply chains are extremely complex, and manual assessment for a real product is rarely possible. Instead, such MF calculations are performed using the existing LCA-based analytical framework. However, to estimate the MC rather than the MF of the product, the non-incorporated flows have to be excluded from the supply. Yet, such flows are not distinguished within the traditional LCA model and the existing LCI databases.

We now present the general analytical approach of estimating the MC of a product within the LCA framework, given that the non-incorporated material flows are distinguished. Later, in Sections 3 and 4, we present a way to filter such flows and estimate the MC of actual products within existing LCI databases.

2.3 | Mathematical model

Here, we present a general analytical model describing our method of MC estimation based on the computational structure of LCA as described by Heijungs and Suh (2002). The general idea behind our proposed approach to obtain the MC of a given product from a given LCI database is as follows. First, we filter out the non-incorporated material flows from all activities along the entire supply chain, including both intermediate and elementary exchanges. Second, we sum up the quantities of the substances of interest present in the remaining flows.

Let us denote the existing square *technosphere matrix* that describes the intermediate flows within the economic system as A. More specifically, each column of the matrix describes the inputs (negative numbers) required and the outputs (positive numbers) delivered by each unit process for an economic production system where multi-functionality (see Section 4.2) has been resolved. Hence, each column is a distinct process in the economy that uses certain outputs of the other processes and delivers its own output (see *Section SI1 of Supporting Information or SI for the clarifying examples of such matrices*). Additionally, B stands for the *intervention (biosphere) matrix*, which describes the environmental pressures (elementary flows) related to the economic activities (including all the dissipative losses into the environment), and f_k specifies the *final demand* vector related to the single unit of product k.

Then, all the activities in the economy required to deliver the product are given as:

$$s = A^{-1}\ f_k \tag{1}$$

where s is called a *scaling vector*.

Consequently, the reference outputs delivered by each activity to satisfy the final demand are given by the so-called *supply array* (or a *supply vector* sometimes for simplicity):

$$t = \text{ ref}\,(A)\ s \tag{2}$$

where ref(A) is a modification of matrix A where each column contains only one non-zero value—the single reference product quantity of each unit process while the rest of the values (all the inputs) are zeros. Such multiplication allows obtaining actual total outputs for all the activities, given that some unit processes output nonsingular quantities.

Similarly, environmental pressures caused by the supply of the final demand are given by the so-called *inventory vector*:

$$g = Bs = BA^{-1}f_k$$

Let us now define the *modified technosphere matrix* $\tilde{A}$ that preserves only those inputs in A that physically enter the corresponding reference products they are inputs of—the incorporated material flows. This matrix could be obtained as follows:

$$\tilde{A} = A \circ P_A \tag{3}$$

where $\circ$ stands for the Hadamard product (element-wise multiplication) of matrices, and P_A is the *material filtering matrix* which either removes the non-material inputs ($p_{ij} = 0$) or specifies which fraction of the input i is physically incorporated into the reference product of the process j ($0 < p_{ij} \leq 1$) in the technosphere matrix A. The cells of the matrix P_A corresponding to the reference products' cells of A are all set to 1 (see Section 2.2 above).

Similarly, we define the *modified biosphere matrix* $\tilde{B}$ as a modification of B that preserves the incorporated (into the reference products) elementary flows only, $\tilde{B} = B \circ P_B$, where P_B is the analogous material filtering matrix for the biosphere matrix, and it filters out the non-incorporated losses that occur during material extraction from the environment. Determining both filtering matrices (P_A and P_B) is the most challenging and crucial part of our method's implementation for real product systems and is described in Section 3.

Accordingly, we can now obtain the *modified scaling vector*: $\tilde{s} = \tilde{A}^{-1} f_k$.

Now, the content of the materials in the reference product k can be estimated either using the *modified (incorporated) inventory vector*:

$$\tilde{g} = \tilde{B}\ \tilde{s} = \tilde{B}\,\tilde{A}^{-1} f_k, \tag{4}$$

or the modified (incorporated) supply array:

$$\tilde{t} = \text{ref}\left(\tilde{A}\right)\ \tilde{s} = \text{ ref}\left(\tilde{A}\right)\ \tilde{A}^{-1} f_k, \tag{5}$$

where $\tilde{g}$ describes the elementary material flows constituting the reference product k (applicable to natural materials) while $\tilde{t}$ describes all the intermediate material flows that are incorporated in the final product k (applicable to both natural and synthetic materials).

When these modified vectors are used for MC estimation, several aspects related to potential double-counting of mass, unit conversion, and material aggregation should be considered. The *material selection and aggregation functions* that formalize the approach to these challenges are defined and described in Section SI7 of SI.

Analogous derivations allow estimating the total MF of the material for the product if the inventory vector g and the same material selection functions are used. This can then be compared to the MC of the product to obtain the NIMF of a product. The supply array t can be used to estimate the MF as well, but it is reasonable for synthetic materials only as it will not account for the natural material dissipation during the extracting activities (see the crude oil example in Table S1 of SI).

JOURNAL OF INDUSTRIAL ECOLOGY WILEY

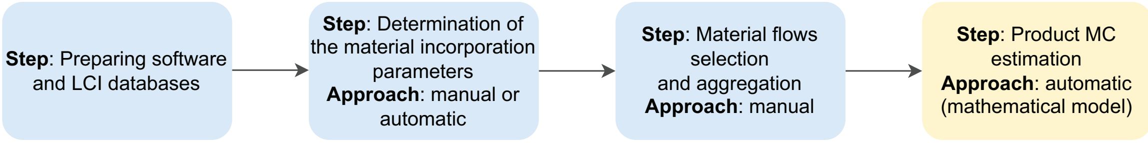

FIGURE 3 Major steps that need to be conducted using the life cycle assessment (LCA) software to estimate the material composition (MC) of the selected product from a life cycle inventory (LCI) database.

For an illustrative example of what the proposed model delivers in estimating the MC of copper and plastic for the simplified laptop manufacturing supply chain from Figure 2, see Section SI1 of SI.

3 | IMPLEMENTATION

The above-mentioned laptop supply chain (Figure 2) is simple enough to perform the required calculations manually. Nevertheless, to estimate the MC of real products, complex supply chains described in LCI databases have to be processed. In this section, we briefly list the steps that will be required from a practitioner to implement the proposed method of product MC estimation in practice while elaborating on the details behind each step in the corresponding sections of SI:

1. Software and LCI database preparation (Section SI8-A).
2. The underlying LCI database is modified using the corresponding material filtering matrices that separate the non-incorporated flows. In practice, we have considered and proposed two approaches for such modification: manual and algorithmic (Sections SI8-B and SI8-C). The simplest filtering algorithm scans the whole LCI database for all the activities and all the exchanges, and it automatically assigns the value of zero (0) to the corresponding "Incorporated" parameter if the exchange's name (process input or output) contains any keyword from the previously prepared *avoid list*, and the value of one (1) otherwise.
3. Manual definition of the material selection and aggregation functions (Section SI8-D). In general, such selection implies assigning specific materials of interest (e.g., plastic or copper) to the corresponding producing unit processes (for synthetic/natural materials) or elementary flows (for natural materials) in the LCI databases that supply such materials. The selected values can be further summed to obtain the MC estimates for more aggregated material categories.
4. As a result, to implement the proposed approach, three preparatory steps must be conducted before the fourth step: calculating the MC of a product based on the mathematical model presented above using the selected software and database (see Figure 3).

An open-source code developed within this study that allows practitioners to perform the proposed product MC estimations has been made accessible (https://doi.org/10.5281/zenodo.5554889). The code implements all the algorithmic steps described in this section and the following case study using the Activity Browser (Steubing et al., 2020) and Brightway (Mutel, 2017) software frameworks.

4 | CASE STUDY

In this chapter, we apply the above-described algorithm of the MC estimation for several products and materials in the widely used ecoinvent LCI database and assess the accuracy of the results. First, however, we introduce the structure of the database itself and overlay it with the previously introduced material flow classification.

4.1 | Ecoinvent database

Ecoinvent is a widely used LCI database containing around 18,000 activities in version 3.6, which is used in this study (Wernet et al., 2016). These activities define all the *inputs* and *outputs* related to unit processes (UPR) describing the production, use, consumption (market), or treatment of goods and services.

Most ecoinvent activities describe the production of goods and services or the treatment of wastes (so-called *transforming* activities). Between two producing activities, there is typically a market activity that acts as a consumption mix for activities that produce the same product within a

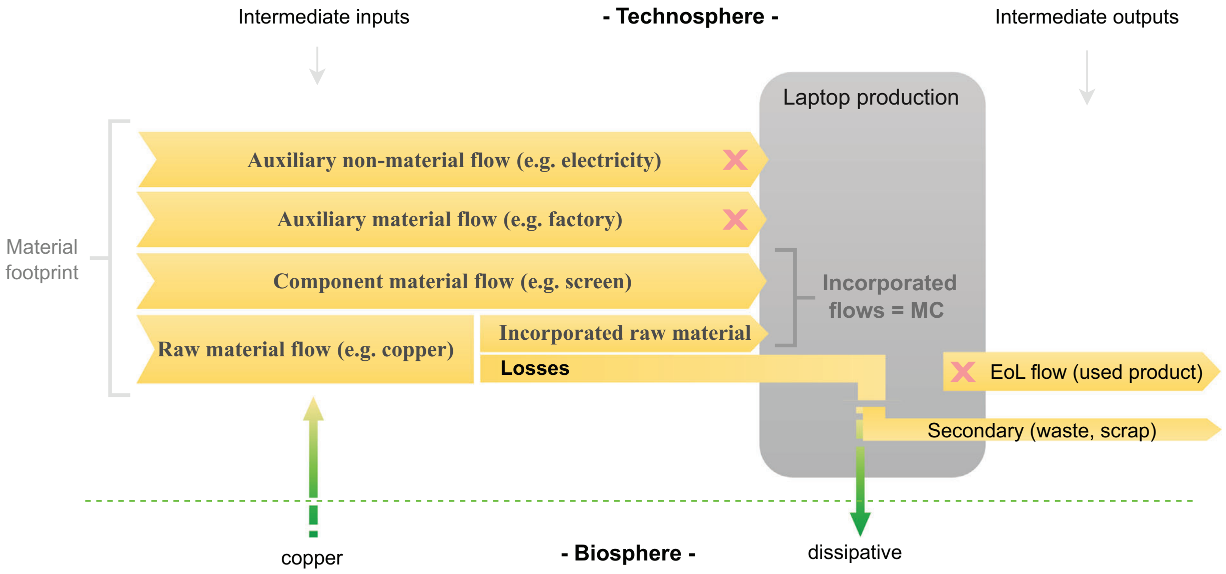

FIGURE 4 Description of the process inputs and outputs within the ecoinvent framework for a single laptop production activity. Distinguishes incorporated (e.g., components, raw materials) and non-incorporated material inputs (auxiliary, dissipative losses, manufacturing losses). X sign denotes the ecoinvent exchanges we want to filter out from the technosphere matrix. Secondary outputs are left as they correct the material inputs for process losses. MC, material composition.

TABLE 1 Materials considered in the case study, along with the corresponding ecoinvent activities.

Material	Activity in ecoinvent
Cu	*market for copper*
Al	*market for aluminum* (*cast alloy* + *wrought alloy* OR *primary*)
Ta	*market for tantalum, powder, capacitor-grade*
Plastic	29 plastics types (see SI3)

certain region (so-called transferring activities). Such market activities allow accounting, for instance, for transportation, retail-related interventions (e.g., cooling), and losses.

The intermediate exchanges of a specific ecoinvent production activity could be categorized into: (1) material and non-material inputs (positive), some of which are incorporated into the product, and (2) outflows of the activities (negative waste flows, used by-products outflows, scrap outflows). To obtain the MC using the above-proposed computational approach applied to the ecoinvent database, we first want to filter out the non-incorporated material flows by adjusting the following three types of exchanges in the technosphere matrix of the ecoinvent to obtain the modified technosphere matrix:

a. Auxiliary positive inputs that are not incorporated in the reference product → filter out ("incorporated" parameter equals zero)
b. Partially incorporated inputs → adjust while accounting for the process and dissipative losses ("incorporated" parameter between 0 and 1)
c. Negative end-of-life (EoL) material burden that is often included in the exchanges of the producing activities of ecoinvent as well → filter out ("incorporated" parameter equals zero)

Unfortunately, in ecoinvent, the latter EoL flows only rarely appear as a distinct *used* product output that could be excluded and, most of the time, are combined with the negative process and dissipative losses. This will be discussed in Section 6 in more detail, but it is currently impossible to separate the EoL flows from the losses in the current ecoinvent version. Hence, both were filtered out.

We present an exemplifying diagram where a simplified case of the copper flows related to the laptop manufacturing activity is considered and where each of the three ecoinvent-specific non-incorporated flow types (a–c) is depicted (see Figure 4). Compared to the previous diagram (Figure 2), it focuses on a single process structure in ecoinvent rather than the whole supply chain.

4.2 | Ecoinvent models

Economic activities are often multi-functional, which means that the activity fulfills several functions at once, such as co-producing several products, treating several products, or recycling one product while producing another. Multi-functionality can be resolved among others through system expansion or partitioning, and since version 3 of ecoinvent, three system models have been developed that deal differently with multi-functionality: the "allocation, cut-off by classification" (*cut-off*), the "allocation at the point of substitution" (APOS), and the "substitution, consequential, long-term" (*consequential*) models. Our study will consider and compare the application of our proposed methodology within each of these.

4.3 | Case study description

To validate the proposed algorithm, we tailor it to the ecoinvent 3.6 LCI database and compare its results for various products and materials with the existing sources. In particular, we consider three natural and one synthetic material: copper, aluminum, tantalum, and plastic. At the same time, we run the code for three ecoinvent products (manufacturing activities): a laptop, a passenger vehicle, and a refrigerator. For each material-product pair, we compare the resulting MC estimations delivered by our algorithm with those from the existing sources (physical surveys, reports, studies, etc.; see Section 4.6 for results).

For each product and the material, two independent sources have been found in the literature to obtain an average theoretical (accepted) MC of the product (see SI4 for the reference sources used). Considering these as more accurate, we specifically chose sources that incorporate recycling, chemical treatment, original manufacturer's data, or physical dismantling in their research processes instead of those that use other sources indirectly. Only for the tantalum content in a passenger vehicle, we could not find a second source. Here, the MC of a product is given as a weight ratio (percentage) occupied by a specific material.

Additionally, we compare the performance of the inventory and the supply array-based approaches as well as the different ecoinvent database models (cut-off, APOS, and consequential).

4.4 | The avoid list of keywords

Here, the algorithmic filtering of the non-incorporated flows in ecoinvent is used since the database is too extensive to manually assign all the parameters for all the exchanges.

The list of keywords to avoid (as being related to either auxiliary, secondary, or EoL flows) when scanning the database is set to the following:

"treatment," "water," "waste," "container," "box," "packaging," "foam," "electricity," "factory,", "adapter," "oxidation," "construction," "heat," "facility," "gas," "freight,""mine," "infrastructure," "conveyor," "road,", "building," "used,", "maintenance," "transport," "moulding," "mold," "wastewater," and "scrap."

We further describe how this list was defined and its sensitivity to selected products and materials of interest in Section SI6 of SI.

4.5 | Material selection and aggregation

For this case study, we consider plastic content in different products. It has been discussed in the Implementation section that the synthetic materials of interest have to be linked to the related material-producing activities (unit processes) in the LCI database for the supplied array-based algorithm to select and accumulate the total material flows.

Yet, dozens of different plastics in various forms are reported in the ecoinvent database. Hence, all such plastics-related activities have been automatically categorized between different plastic types by scanning the ecoinvent database for specific keywords like PET, PVC, and so on. All found activities are assigned to the corresponding plastic types. Then, the related production activities for three natural materials (Al, Cu, and Ta elements) were identified and linked. As a result, a complete list of ecoinvent activities related to these four materials of interest has been selected for the supply array-based MC estimation (see Table 1). Various nuances related to this work, including the market activities and the double-counting issue, are described in detail in SI3.

4.6 | Results

As a result, comparing the performance of our two algorithms across all four products and three possible database models, on average, the supply array-based algorithm applied on the consequential model of the ecoinvent allowed estimating the MC of metals with the lowest deviation (26% relative error and 1.1% absolute error on average) from the theoretical MC of the products (see SI4 for the calculations and reference sources used).

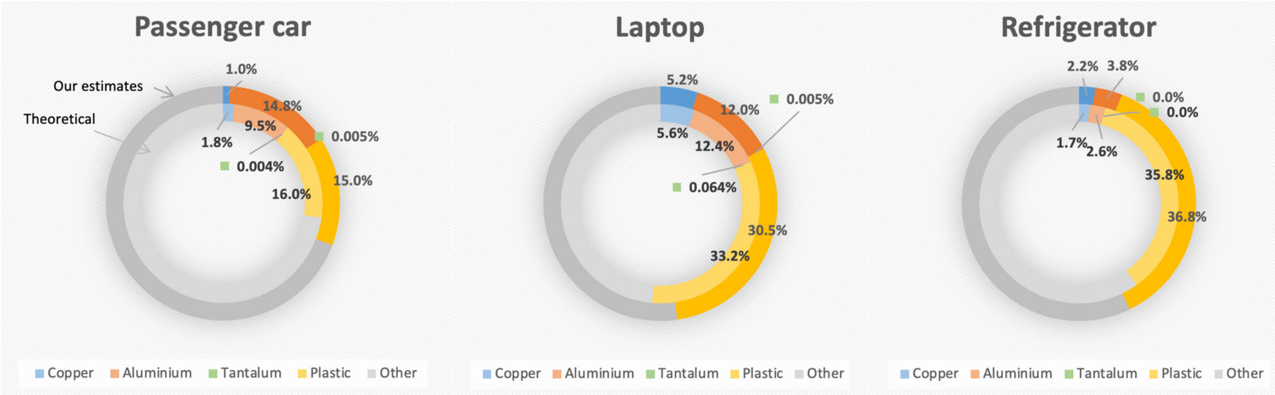

FIGURE 5 Results for three different consumer goods for the supply array-based approach applied on the consequential model of the database. The material composition of products is given relative to the total mass of a product. Underlying data are available in Sheet1 of Supporting Sheets.

TABLE 2 Resulting multipliers to obtain the material footprint (MF) of a product given its material composition (MC).

Product/material	Cu	Al	Ta	Plastic
Passenger car	1.58	1.14	1.00	1.33
Laptop	2.29	1.29	1.00	2.02
Refrigerator	1.07	1.04	–	1.60

Note: Tantalum is not present in a refrigerator.

The results for three different consumer goods upon applying the supply array-based approach to the consequential model of the database are presented (see Figure 5).

Additionally, since the material dictionary was based on a highly detailed categorization of plastics types, values for specific plastics have been obtained along with the case study (see SI5).

4.7 | Material footprint versus material composition

The proposed method allows for distinguishing the MC of a product versus its total MF. Table 2 presents the resulting multipliers to obtain the MF of the material given its MC; the difference suggests the corresponding NIMF as well.

5 | DISCUSSION

In general, the supply array-based algorithm developed within this study proved to be quite accurate for estimating the MC of products reported in the ecoinvent database, while the consequential model of the ecoinvent tends to perform best.

When using the inventory vector-based approach to estimate the MC in the cut-off model of the database, the material impacts (elementary flows) of the secondary (e.g., recycled) material inputs will be cut off due to the nature of this model. Hence, the inventory vector should be used with other database models to avoid possible MC underestimation. Meanwhile, using the supply vector-based approach to source the MC estimates from the corresponding market activities (with any model of the database) eliminates this problem because such activities already accumulate both primary and secondary flows. Additionally, if one is interested in the relative contribution of the secondary versus primary material used in the production, specific inputs into such market activities can be compared in the resulting supply vector.

The supply array-based approach is reasonably applicable to both (natural and synthetic) materials if proper material-producing activities are selected and aggregated in the supply chain as representative of the materials of interest (see Section 4.5). Meanwhile, using the inventory vector-based approach to estimate the MC of synthetic materials is rarely meaningful (e.g., estimating plastic content through crude oil content, see Table S1 of SI), and we suggest applying it to natural materials only.

The inventory vector accounts for environmental exchanges (i.e., elementary flows) along the whole supply chain. Hence, whenever there is a substance that is reported as a dissipative flow in any of the material incorporating activities in the product's upstream supply chain, that will decrease the total mass of that substance being carried by that activity into the final product and would make the resulting MC estimation more accurate. Nevertheless, such elementary outflows were not found to be reported in ecoinvent for the processes and substances explored in this study, and yet, they could be the most reasonable place within the LCI databases to report and account for the dissipative losses to the environment, as has been previously suggested (Beylot et al., 2020)

Moreover, our approach allows for the automatic assessment of the gap between the MC and the total MF of the product manufacturing. This is quite significant for some materials and products. For instance, the non-incorporated copper and plastic material burden of a laptop is more than twice as large as its material contents (see Table 2). Interestingly, the MF of tantalum in a laptop or a passenger vehicle is not different from the MC, which might appear unrealistic. This can be because, in the ecoinvent database, tantalum is reported as being used only in capacitors that, in turn, are used mostly in PCBs (e.g., in laptops), which, in turn, are not reported as part of any upstream auxiliary inputs (e.g., laptops used at the factory that manufactures laptops) for the products of our interest. We look forward to the corresponding improvements in the future LCI databases.

6 | LIMITATIONS AND PROSPECTS

Here, we list some of the limitations and areas of possible future improvement related to this work.

The avoid list sensitivity to products and materials of interest

The avoid list used to filter material flows is applicable for a general product in the ecoinvent. Still, it depends on the material of interest and has to be manually adjusted each time. For instance, water should not be excluded if one is interested in the water content. On the other hand, a practitioner should be prepared for accidental labeling of certain inputs as auxiliary, such as with the “sodium hydroxide, without water” in the refrigerator that contains the “water” keyword from the avoid list.

Material composition of infrastructure

If the MC of the auxiliary product itself is explored (e.g., Cu content in the factory building), then the algorithm has to target the factory’s production activity (not its market activity) when the automatic assignment of the “incorporated” parameters is applied. Otherwise, since all the production inputs into the market activity will be filtered out automatically as an auxiliary, the estimate will not be meaningful.

Proportional incorporation of complex materials

The fact that a single material incorporation parameter (between 0 and 1) is given per each process input assumes uniform incorporation even if several sub-materials are part of the same input. This can be seen as unrealistic for some processes, for example, ore processing where sub-material (rock and metal content) are processed and incorporated differently, or the datasets for chemical compounds where non-active ingredients are not part of the reference outflow. Yet, in many cases, proper assignment of process and dissipative losses can tackle the issue. Alternatively, in more developed versions of our algorithm, multidimensional material-dependent incorporation parameters can be introduced wherever materials are not processed and incorporated proportionally.

System boundaries of the material footprint

The MF of products in this study has been constrained within the cradle-to-product life cycle stages. This allows a meaningful comparison of the MF with the MC, which is, by definition, an accumulation of incorporated material flows up until the product delivery stage. Nevertheless, it should be acknowledged that the MF of products can be defined along various system boundaries and could include the EoL material impacts (see Section 2.1).

Lack of variation of product types and models in LCI databases

It must be noted that our approach does not allow us to distinguish between the variety of models and brands of the same type of product in the real world. Moreover, not all materials and products are presented in the existing LCI databases, and yet, they are developing quickly and contain many more materials than the limited number that was selected for this study.

Lack of common EoL reporting protocols in ecoinvent

The absence of a standardized reporting protocol for production outflows in ecoinvent compromises the accuracy of the proposed MC estimation approach. Specifically, certain products (e.g., Al for passenger car production) report manufacturing losses separately from used product outputs, while others (e.g., Cu in fridge production) combine these under a common outflow (that is usually equal to the total input mass of the material). This lack of distinction hinders the calculation, leading to a slight overestimation of MC. When the used product's EoL outflow is separate and contains the material of interest (e.g., Al in engines), manufacturing losses can be inferred from scrap and waste flows, allowing correction for more accurate MC estimates. Adjusting material incorporation allows for manual specification of losses if known. Additionally, when the total product weight is reported in the ecoinvent, dividing it by the total mass of non-auxiliary inputs can provide an estimate for the average material loss rate, although unit variations pose a challenge.

Lack of product and material variation in our case study

The primary aim of this methodological research was to demonstrate the suitability of existing LCI data for estimating product MC and to assess the proposed algorithm's accuracy. Consequently, a limited number of products and materials with known theoretical MC values were considered for verification. While the algorithm is material-independent, the case studies focused only on abiotic substances. The openly accessible algorithm and Python script enable practitioners to obtain MC values for other products and materials with access to the LCI database.

The challenge of mass balance preservation in LCI databases

Finally, we want to mention that the mass balances are not strictly preserved in the LCI databases. This is caused by the way the multi-functionality problem is approached in such databases (often using economic allocation). Future studies have to explore how this effect varies between different LCI databases.

7 | CONCLUSIONS AND RECOMMENDATIONS

The developed method presents promising results in estimating the MC of various products without reliance on time and cost-intensive approaches such as chemical analysis, physical dismantling, or manual data consolidation from dispersed sources. The most accurate results are delivered when the supply array-based approach is applied to the consequential LCI databases.

Additionally, this research allowed us to compare a product's MC with its NIMF. It has been shown that the NIMF is rather significant for some products and materials. This suggests that, for some materials, the recycling policy should also consider resource recovery from upstream supply chains instead of focusing solely on recycling the final products.

Based on our experience with the recent versions of ecoinvent, the following developments of the database are suggested to allow much more reliable estimates. First, having the EoL material burden from *used* products specified separately from the process losses (i.e., scarp and waste flows) within each of the production processes (currently, usually mixed under common outputs) would allow to correct for such losses and improve the accuracy of the MC estimations (see Section 4.1 and Figure 4 for an example). Second, the material incorporation rate parameter given for all the inputs into the production activities of the LCI databases would enrich the potential of the databases and allow for systematic and accurate estimation of the MC of products. Such parameters could be initially assigned by the corresponding contributors to the LCI databases during their assembly so that the end-users would not need to assign them themselves (either algorithmically or manually) without specific expert knowledge. Additionally, the total product weight reported for each production activity would allow more accurate estimates of the relative content. Simultaneously, such development would directly contribute to the official provisions on the elemental composition of products and waste flows that are set by the European Commission—Joint Research Centre (2010).

While the accuracy of the presented algorithm was tested on the ecoinvent database, it is universally applicable to any LCI database since they share a common LCA-based framework. However, the algorithm's specific implementation will depend on the particular application database and may require customization to accommodate its features, such as the naming of unit processes, types of intermediate flows, level of detail, and other factors.

As a result of this work, a Python code that allows to automatically specify the material incorporation parameters for the ecoinvent exchanges and to estimate the MC of a material of interest for any of the ecoinvent products is published at: https://doi.org/10.5281/zenodo.5554889 (Amatuni, 2023).

To conclude, this study proposes an accurate and accessible approach for estimating the MC of products and suggests several ways to improve current LCI databases, which could solve the underlying challenges and limitations.

ACKNOWLEDGMENTS

This paper results from the three-year research project PANORAMA (2019-2022) funded by the European Institute of Innovation and Technology (EIT). We acknowledge Arnold Tukker (Leiden University) for acquiring the funding and promoting work on the project. We further acknowledge Daniel de Koning (Leiden University at the time of this work) for his help with our Activity Browser-based calculations. We finally acknowledge Zhijie Li (Leiden University at the time of this work) for her help with classifying the plastics types.

CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available on GitHub at https://doi.org/10.5281/zenodo.5554889

ORCID

Levon Amatuni https://orcid.org/0000-0002-8125-0858
Bernhard Steubing https://orcid.org/0000-0002-1307-6376
Tales Yamamoto https://orcid.org/0000-0001-8392-0002

REFERENCES

Amatuni, L. (2023). levonamatuni/material-composition-lca: V0.12-alpha (v0.12-alpha). Zenodo. https://doi.org/10.5281/zenodo.7521684

Beylot, A., Ardente, F., Sala, S., & Zampori, L. (2020). Accounting for the dissipation of abiotic resources in LCA: Status, key challenges and potential way forward. *Resources, Conservation and Recycling*, *157*(February), 104748. https://doi.org/10.1016/j.resconrec.2020.104748

Ciroth, A., & Burhan, S. (2021). Life cycle inventory data and databases. In A. Ciroth, & R. Arvidsson (Eds.) *Life cycle inventory analysis* (pp. 123–147). Springer. https://doi.org/10.1007/978-3-030-62270-1_6

Dionisio, K L., Phillips, K., Price, P S., Grulke, C M., Williams, A., Biryol, D., Hong, T., & Isaacs, K K. (2018). Data descriptor: The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products. *Scientific Data*, *5*, Article 180125. https://doi.org/10.1038/sdata.2018.125

European Commission—Joint Research Centre—Institute for Environment and Sustainability. (2010). *International reference life cycle data system (ILCD) handbook : Specific guide for life cycle inventory data sets. EUR 24709 EN*. European Commission. https://doi.org/10.2788/39726

Heeren, N., & Fishman, T. (2019). A database seed for a community-driven material intensity research platform. *Scientific Data*, *6*, 1–10. https://doi.org/10.1038/s41597-019-0021-x

Heijungs, R., & Suh, S. (2002). *The computational structure of life cycle assessment* (Vol. 11). Springer. https://doi.org/10.1007/978-94-015-9900-9

Hoekstra, R., & Van Den Bergh, J. C. J. M. (2006). Constructing physical input-output tables for environmental modeling and accounting: Framework and illustrations. *Ecological Economics*, *59*(3), 375–393. https://doi.org/10.1016/j.ecolecon.2005.11.005

Horta Arduin, R., Mathieux, F., Huisman, J., Blengini, G. A., Charbuillet, C., Wagner, M., Baldé, C. P., & Perry, N. (2020). Novel indicators to better monitor the collection and recovery of (critical) raw materials in WEEE: Focus on screens. *Resources, Conservation and Recycling*, *157*(March), 104772. https://doi.org/10.1016/j.resconrec.2020.104772

ISO. (2006). Environmental management - Life cycle assessment - Principles and framework *ISO 14040:2006*. International Organization for Standardization. https://www.iso.org/standard/37456.html

Jensen, J. P., & Remmen, A. (2017). Enabling circular economy through product stewardship. *Procedia Manufacturing*, *8*, 377–384. https://doi.org/10.1016/j.promfg.2017.02.048

Lettenmeier, M., Rohn, H., Liedtke, C., & Schmidt-Bleek, F. (2009). Resource productivity in 7 steps: How to develop eco-innovative products and services and improve their material footprint. Wuppertal Spezial. https://nbn-resolving.org/urn:nbn:de:101:1-2010050774 Accessed July 9, 2024

Mostert, C., & Bringezu, S. (2019). Measuring product material footprint as new life cycle impact assessment method: Indicators and abiotic characterization factors. *Resources*, *8*, 61. https://doi.org/10.3390/resources8020061

Mutel, C. (2017). Brightway: An open source framework for life cycle assessment. *The Journal of Open Source Software*, *2*, 236. https://doi.org/10.21105/joss.00236

Nakamura, S., Kondo, Y., Matsubae, K., Nakajima, K., & Nagasaka, T. (2011). UPIOM: A new tool of mfa and its application to the flow of iron and steel associated with car production. *Environmental Science and Technology*, *45*(3), 1114–1120. https://doi.org/10.1021/es1024299

Nakamura, S., & Nakajima, K. (2005). Waste input-output material flow analysis of metals in the japanese economy. *Materials Transactions*, *46*(12), 2550–2553. https://doi.org/10.2320/matertrans.46.2550

Oguchi, M., Murakami, S., Sakanakura, H., Kida, A., & Kameya, T. (2011). A preliminary categorization of end-of-life electrical and electronic equipment as secondary metal resources. *Waste Management*, *31*(9–10), 2150–2160. https://doi.org/10.1016/j.wasman.2011.05.009

Ohno, H., Sato, H., & Fukushima, Y. (2018). Configuration of materially retained carbon in our society: A WIO-MFA-based approach for Japan. *Environmental Science and Technology*, *52*(7), 3899–3907. https://doi.org/10.1021/acs.est.7b06412

Passer, A., Lasvaux, S., Allacker, K., De Lathauwer, D., Spirinckx, C., Wittstock, B., Kellenberger, D., Gschösser, F., Wall, J., & Wallbaum, H. (2015). Environmental product declarations entering the building sector: Critical reflections based on 5 to 10 years experience in different European countries. *International Journal of Life Cycle Assessment*, *20*, 1199–1212. https://doi.org/10.1007/s11367-015-0926-3

Saurat, M., & Ritthoff, M. (2013). Calculating MIPS 2.0. *Resources*, *2*, 581–607. https://doi.org/10.3390/resources2040581

Schmidt-Bleek, F. (1994). MIPS: Ein neues ökologisches Maß. In *Wieviel umwelt braucht der mensch?* (pp. 97–141). Birkhäuser Basel. https://doi.org/10.1007/978-3-0348-5650-8_4

Singh, J., & Ordoñez, I. (2016). Resource recovery from post-consumer waste: Important lessons for the upcoming circular economy. *Journal of Cleaner Production*, *134*, 342–353. https://doi.org/10.1016/j.jclepro.2015.12.020

Steubing, B., De Koning, D., Haas, A., & Mutel, C. L. (2020). *The Activity Browser—An open source LCA software building on top of the brightway framework*. Software Impacts. https://doi.org/10.1016/j.simpa.2019.100012

Stigson, B., Madden, K., Young, R., Brady, K., & Hall, J. (2006). *Eco-efficiency learning module*. World Business Council for Sustainable Development(WBCSD). https://www.wbcsd.org/Projects/Education/Resources/Eco-efficiency-Learning-Module

Teehan, P., & Kandlikar, M. (2013). Comparing embodied greenhouse gas emissions of modern computing and electronics products. *Environmental Science and Technology*, *47*(9), 3997–4003. https://doi.org/10.1021/es303012r

UNEP. (2021). *The use of natural resources in the economy: A global manual on economy wide material flow accounting*. https://www.resourcepanel.org/reports/global-manual-economy-wide-material-flow-accounting

Wäger, P. A., Hischier, R., & Widmer, R. (2015). The material basis of ICT. In *ICT innovations for sustainability* (vol. 310, pp. 209–221). Springer International Publishing. https://doi.org/10.1007/978-3-319-09228-7

Webster, M. (2022). Merriam Webster dictionary. In *Merriam Webster.com dictionary*. https://www.merriam-webster.com

Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., & Weidema, B. (2016). The ecoinvent database version 3 (part I): Overview and methodology. *International Journal of Life Cycle Assessment*, *21*, 1218–1230. https://doi.org/10.1007/s11367-016-1087-8

Wiedmann, T. O., Schandl, H., Lenzen, M., Moran, D., Suh, S., West, J., & Kanemoto, K. (2015). The material footprint of nations. *Proceedings of the National Academy of Sciences of the United States of America*, *112*(20), 6271–6276. https://doi.org/10.1073/PNAS.1220362110/-/DCSUPPLEMENTAL

Wiesen, K., Saurat, M., & Lettenmeier, M. (2014). Calculating the material input per service unit using the Ecoinvent database. *International Journal of Performability Engineering*, *10*(4), 357–366.

Williams, E. D., Ayres, R. U., & Heller, M. (2002). The 1.7 kilogram microchip: Energy and material use in the production of semiconductor devices. *Environmental Science, & Technology*, *36*(24), 5504–5510. https://doi.org/10.1021/es025643o

Zimmermann, T., & Gößling-Reisemann, S. (2013). Critical materials and dissipative losses: A screening study. *Science of the Total Environment*, *461-462*, 774–780. https://doi.org/10.1016/j.scitotenv.2013.05.040

SUPPORTING INFORMATION

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

How to cite this article: Amatuni, L., Steubing, B., Heijungs, R., Yamamoto, T., & Mogollón, J. M. (2024). Deriving material composition of products using life cycle inventory databases. *Journal of Industrial Ecology*, *28*, 1060–1072. https://doi.org/10.1111/jiec.13538