Methodology for the Construction of Global Multi-Regional Hybrid Supply and Use Tables for the EXIOBASE v3 Database

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Summary

This article describes the algorithm that has been developed within the European Union (EU) FP7 project DESIRE for the construction of the EXIOBASE multiregional hybrid supply and use tables (MR-HSUTs) version 3. The tables include 43 countries plus five rest-of-the-world regions and are built for the period 2000–2011. MR-HSUTs are compiled in mixed units, that is, tangible goods in mass units, intangible energy flows in terajoules, and, finally, services in euros. The article summarizes the various steps of the developed procedure, from data collection until the final supply and use tables. It will be shown how several disconnected data sets with varying quality are harmonized so as to build an effective analytical database that can be used for several types of analyses, such as life cycle assessment, total material requirement, material intensity per product service, carbon footprint, and so on.

Introduction

Multiregional supply and use tables (MR-SUTs) describe the behavior of producers and consumers in current economies. The latter are, in turn, interconnected with one another covering all the transactions occurring worldwide. Therefore, MR-SUTs are a robust tool for a wide range of analyses, covering environmental, social, and economic spheres. The scale of the analyses can be sectorial so as to be national or global.

This paper describes the procedure that has been developed to build global multiregional hybrid supply and use tables (MR-HSUTs) in the European Union (EU) FP7 project DESIRE. These data sets are used for the EXIOBASE database v3 (Tukker et al. Forthcoming). The presented methodology is a further improvement of what we have developed in the EU FP7 project CREEA (Schmidt et al. 2012; Merciai et al. 2013; Wood et al. 2015), which, in turn, is based on outcomes of the EU FP6 project FORWAST (Schmidt et al. 2010). The term *hybrid* is here used to indicate the mixed-unit framework with three layers of the supply and use tables (SUTs), namely a mass layer (flows with a physical mass: products and waste material), an energy layer (electricity and heat), and a monetary layer (services).

Other global multiregional input-output (I-O) data sets have been published so far (Andrew and Peters 2013; Lenzen et al. 2012, 2013; OECD 2015; Timmer et al. 2015; Tukker et al. 2009, 2013). All these databases, although adopting different classifications, methods, etc. (Tukker et al. Forthcoming; Wood et al. 2014), share the common principle of accounting the transactions between activities of the world economies uniquely in monetary terms.

At the same time, many I-O tables (IOTs) accounted in mass units have been published for many countries (Gravgård-Pedersen 1999; Hoekstra 2005; Konijn et al. 1995; Mäenpää and Muukkonen 2001; Nebbia 2000; Stahmer et al. 1997;

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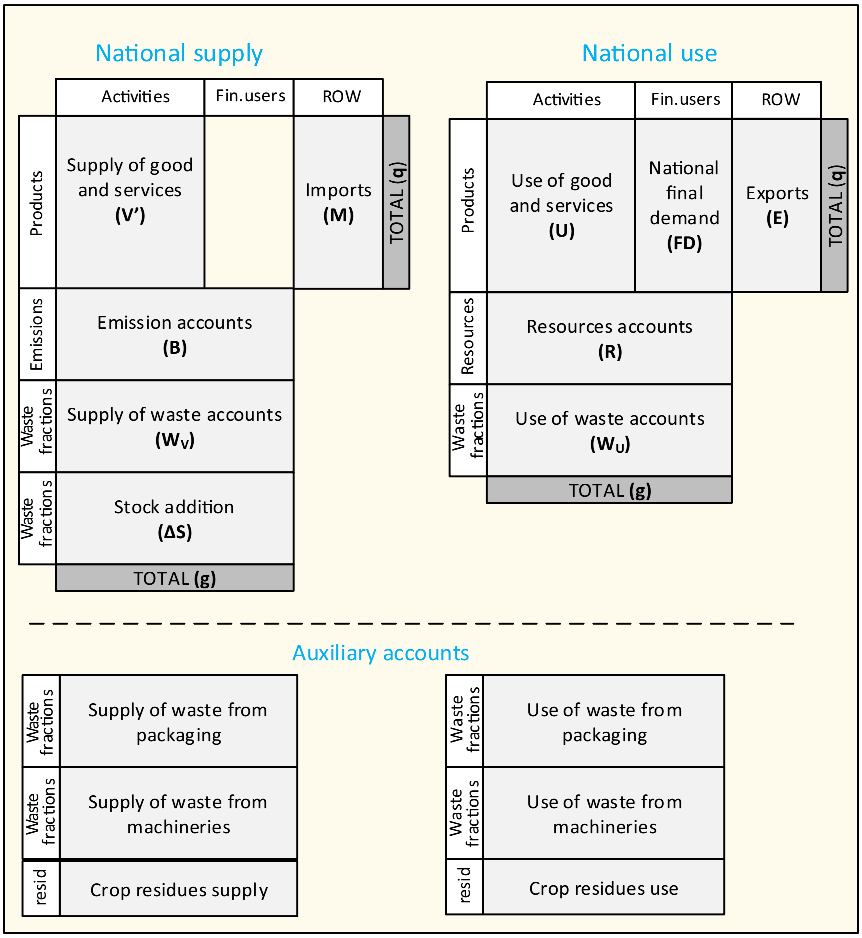

Figure 1 Framework adopted for the construction of national HSUTs (hybrid supply and use tables). Waste treatment services are accounted in the supply and use of good and services (V' and U), while waste accounts show the mass flows linked to these waste treatment services. ROW refers to rest-of-the world. See table 1 for a description of the content of the tables.

Statistisches Bundesambt 2011), but none of them included more than one region. Stahmer (2000) published a multilevel IOTs for Germany, but again it was just for a single region of the world. Schmidt and colleagues (2010), published a mixed-units SUT with two regions, Denmark and EU-27. Therefore, EXIOBASE MR-HSUTs are the first ever compiled and published global multiregional hybrid tables.

Among many others, there is one important advantage of constructing SUTs in different layers, each with different units, and then combining these into a hybrid mixed-units framework (Hawkins et al. 2007; Majeau-Bettez et al. 2016; Merciai and Heijungs 2014; Weisz and Duchin 2006): the possibility within each activity, and for all the products, to perform balances in different units. In our case, we have imposed in the algorithm the mass and energy balances.[1] This assures that a production process has always enough inputs to satisfy its production. Further, there is always consistency between the externalities and the uses of products. For example, the emissions due to the combustion of a kilogram (kg) of specific fuels.

Further, the aggregation of products and activities may hide the presence of different prices per purchaser. When a model is calibrated on monetary tables, the presence of different prices per purchaser may affect the calculated environmental footprints (Merciai and Heijungs 2014). To detect different prices is not possible if only monetary flows are taken into account. Thus, mixed-unit tables can be used to calibrate models whenever the adopted classification may imply different prices per purchaser.

The MR-HSUTs include 43 countries[2] plus five rest-of-world (ROW) regions, and they are calculated annually for the period 2000–2011 in the EU FP7 project DESIRE.

Overview of the Methodology

The framework of the tables (figure 1) is based on the concept of physical supply and use tables (Hoekstra and van den Bergh 2006) as defined in the Systems of Economic and Environmental Accounts (SEEA) (SEEA 2012). Table 1 shows a description of most of the matrices and vectors used in the text.

Matrices are indicated with capital bold letter, while vectors with small bold letters. A matrix with a subscripted Φ indicates

Table 1 List of main matrices and vectors used in the text

Name	*Short description*	*Dimension*	*Description*
V'	Supply table	Products by activities	Show the supply and use of goods and services
U	Use table		
FD	Matrix of domestic final demand	Products by domestic final demand categories	It shows the final demand of national consumers.
M **m**	Matrix of imports Vector of imports (sum)	Products by country/region Products by 1	The matrices refer to a country, therefore sometimes it may be included in the text as M_C where C defines the country. All the matrices of imports (or exports) together give the trade matrix (**N**).
E **e**	Matrix of exports Vector of exports (sum)	Products by country/region Products by 1	
q	Total supplied/used products	Products by 1	Sum of supplied products (domestic and exported) or used products (domestic and imported) for all human activities within a specified period and geographical area
g	Total input/output of activities	1 by activities	Sum of the input or output of activities
A	Coefficient transaction matrix	Products by activities	Subscripts: LCI: Input data with default coefficients T: Dry-matter mass physical coefficient transaction matrix H: Hybrid coefficient transaction matrix
$\mathbf{D}_o$	Default product transfer coefficient matrix	Products by activities	The proportion of the input which is present in the products supplied by the activity. Allowed values ∈ [0,1]. A value ∈ [0,1] indicates that the input is a feedstock material for the activity in the specified proportion.
D	Final product transfer coefficient matrix	Products by activities	The proportion of the input which is present in the products supplied by the activity. Allowed values ∈ [0,1]. This matrix is calculated by the algorithm.
F	Final resource transfer coefficient matrix	Resources by activities	The proportion of the natural resources which is present in the products supplied by the activity. Allowed values ∈ [0,1]. It is initialized by default values $\mathbf{F}_0$.
T	Final waste transfer coefficient matrix	Waste fractions by activities	The proportion of the waste fractions which is present in the products supplied by the activity. Allowed values ∈ [0,1]. It is initialized by default values $\mathbf{T}_0$.
f_{MMR}	Vector of material requirement	Products by 1	Indicates the minimum materials that must be available on the national market to allow given levels of production
N	Physical trade cube	Importer country by product by exporter country	Indicates the bilateral trade between all countries
R	Matrix of resources	Resources by activities	Shows the resources extracted
B	Matrix of emissions	Emissions by activities	Shows the discharged emissions. The emissions can be due to: - Combustion of materials (B_{comb}) - Use of materials (B_{use}) - Supply of products (B_{supply})

Note: LCI = life cycle inventory.

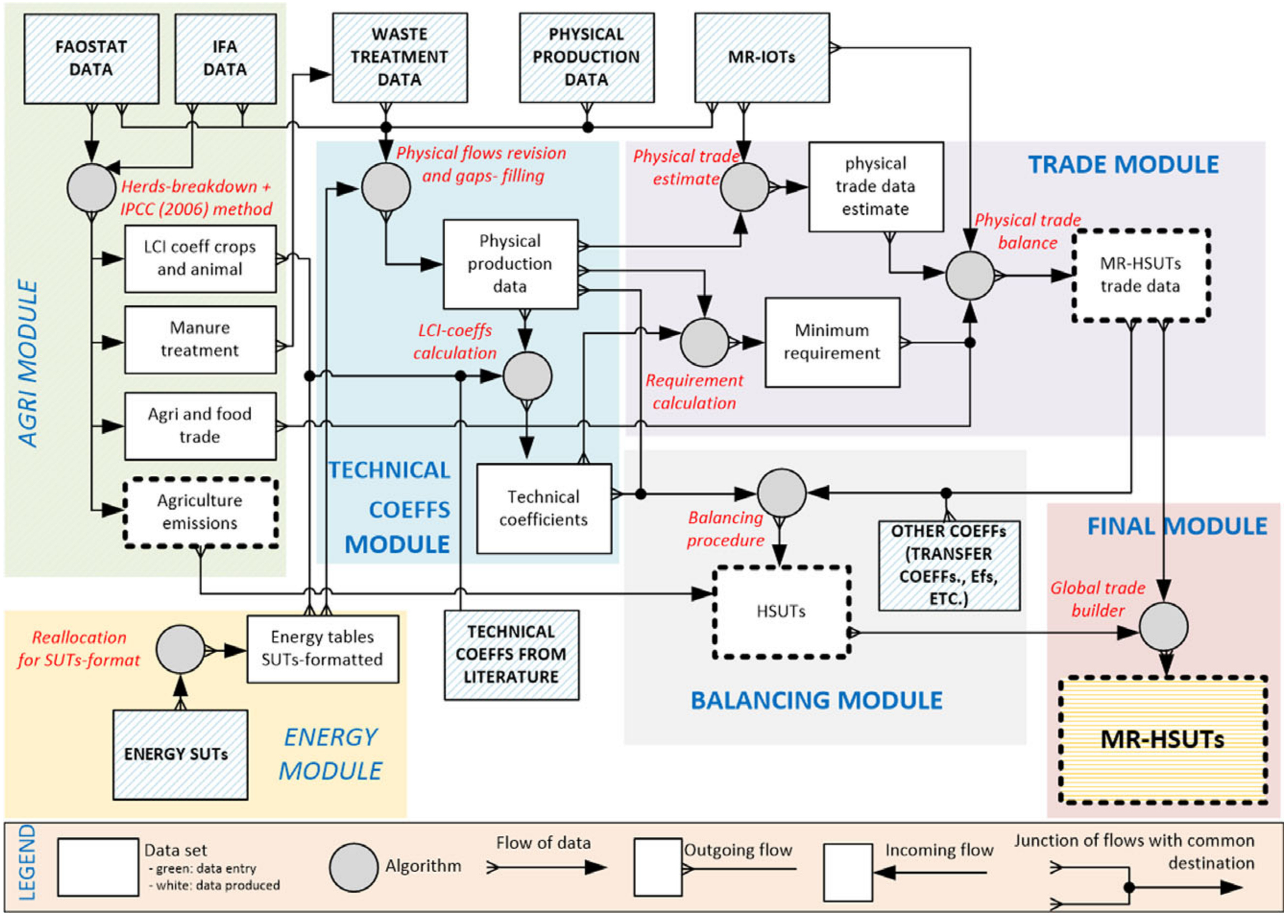

Figure 2 MR-HSUTs algorithm diagram. The algorithm is divided into modules indicated with colored rectangles. The boxes with oblique lines show the collected data, while the white boxes the calculated data. The box with horizontal lines shows the final delivered tables. White boxes with dotted line show the calculated data that are untouched in the algorithm and inserted in the final MR-HSUTs. Coeffs = coefficients; LCI = life cycle inventory; MR-HSUTs = multiregional hybrid supply and use tables; MR-IOTs = multiregional input-output tables; SUTs = supply and use tables.

that is accounted in monetary units, while a subscripted T that is accounted in mixed units, which means that tonne is used for tangible goods, TJ for intangible energy products and euro for services.

The algorithm developed for the construction of MR-HSUTs makes use of several data sources that are harmonized all together in order to get balanced tables. This includes data on: production, trade, physical and energetic technical coefficients, waste treatment, lifetime of products, efficiency factors, weights of animals, moisture content of products, calorific values, etc.

With regard to data collection, databases of international organizations have been prioritized, such as Eurostat, Food and Agriculture Organization of the United Nations (FAO), International Energy Agency (IEA), International Fertilizers Association (IFA), ecoinvent, etc. (EUROSTAT 2015; FAO Statistic Division 2015; IFA 2015; IEA 2015; www.ecoinvent.org). In some cases, national reports have also been used (see Appendix 2 and the References section in Merciai and Schmidt [2016] for an exhaustive list of references). For the monetary flows, the procedures rely on EXIOBASE multiregional monetary SUTs (Stadler et al. 2015).

The algorithm is divided in different modules. There are two types of modules, *sectorial* and *general*. A *sectorial* module is a self-standing block that delivers results to the general part. It is characterized by peculiar functions and is mostly fed by dedicated data source. For example, the agriculture module is sectorial and the FAO is used as main source of data. A *general* module runs generalized procedures for data not included in sectorial modules and implements operations where there is need of working with all the data simultaneously. Figure 2 shows the structure of the whole algorithm. Agriculture and energy modules are sectorial. All the remaining modules are general. The model setup is prepared for adding more sectorial modules in the future to bring in more sectoral detail, data, and modeling.

The core principle underlying the procedure is driven by conservation laws. This implies that for any input, there must be corresponding amounts of outputs. Hence, an input, that is, a product, a natural resource, or a waste flow, can be embodied in other products, disposed of as waste, accumulated as stock or, finally, discharged as emission. At the same, if something is produced, or consumed, there must be input flows that justify such a level of production, or consumption. The data availability will determine which approach needs to be followed and what data must be estimated. The ultimate goal of the MR-HSUTs procedure is indeed that of revising and harmonizing data so that balanced tables are constructed.

With regard to the previous multiregional hybrid tables built in the FP7 project CREEA, which resulted in EXIOBASE v2 (Merciai et al. 2013; Schmidt et al. 2012), many novelties have been included in this new version. An important one is the adoption of homogenous activities classification, which means that each activity supplies the principal production and only co-productions that are technologically linked to it. This is in line with the definition of "kind-of-activity units" (EC et al. 2008, 88–89), that can roughly be defined as sector.

This has implied a consistent improvement when performing the mass and energy balance within the activities. The disadvantage of adopting a different production unit is that a strict correspondence between official monetary and hybrid SUTs is lost in the EXIOBASE v3 database, because the monetary tables follow another approach linked to the establishment (EC et al. 2008, 87), which is close to the concept of industry.

The introduction of the trade module in the algorithm is another major improvement. Physical trade flows are now calculated considering all the different collected data used by the algorithm. In EXIOBASE v2, physical trade was retrieved from the BACI database (Gaulier and Zignago 2010) and kept constant in the physical layer algorithm. Yet, in some cases, the physical trade was highly conflicting with data from other sources. In order to get balanced tables, change on inventories were free to reach any value and this caused unreliable results in many cases. Currently, trade is built starting from monetary trade flows (Stadler et al. 2015) and using various data sources or endogenous estimates.

The reconciliation of data are implemented in the algorithm solving a cross-entropy optimization problem (Golan et al. 1994) that is recognized as a valid adjustment method (Jackson and Murray 2004).

In the following text, we will describe the various modules of the algorithm for the construction of the MR-HSUTs. We have decided to introduce some important formulas included in the algorithm, but not all for objective space limits. A more exhaustive description can be found in Merciai and Schmidt (2016).

We follow a domestic approach with regard to spatial boundary. Only international transportation follows a residency approach (Stadler et al. 2015). Tables are produced in dry-matter (DM) that can be defined as the part of a material that is left after the removal of water. Matrix multiplication (rows by columns), is indicated with a dot ($\cdot$) while element by element product (Hadamard product) is indicated with a star (*). An element of a matrix can be indicated indifferently with subscripted indexes, for example, $\boldsymbol{A}_{ij}$, or con indexes within brackets $\mathbf{A}(i, j)$. A generic row or column of a matrix is indicated with a point as index, for example, $\boldsymbol{A}_{i.}$ or $\mathbf{A}(i, .)$ indicate the *i-th* row of A.

The Agriculture Module

The module aims to determine mass balance for all the agricultural activities. The inputs include, for crop activities, carbon dioxide, minerals, and nutrients from chemical fertilizers and manure, while for livestock the inputs include oxygen for animal respiration, market and nonmarket feed, and grass. The outputs are the productions of activities, that is, harvested crops and animal growth, emissions, and manure excreted. The use of crop residues is taken into account.

Here is a list of tasks accomplished by the module:

- harmonizing FAOSTAT data on agricultural production according to the EXIOBASE classification of agricultural activities. This also means that herds are divided in meat, dairy, and wool systems;
- determining the feed intake of animals and the consequent production of manure;
- determining the use of nutrients by various crops, where nutrients come from both spread manure and chemical fertilizers;
- determining the principal and secondary production of activities, for example, dairy sector may have a coproduction of meat and/or wool. Activity producing live animals may have a coproduction of milk and/or wool. Manure treatment may have a coproduction of fertilizers[3];
- calculating the emissions of agriculture processes, that is, the emissions due to the production of rice (IPCC 2006a), use of fertilizers (IPCC 2006b), enteric fermentation of animals, and treatment of manure (IPCC 2006c);

In this module, all the data regarding agricultural productions, animal stocks, and land use are taken from FAOSTAT (FAO Statistic Division 2015), which is characterized by a high level of completeness with regard to included products in production data and included countries. Data on the use of fertilizers are taken from the IFA (2015). The procedure for the calculation of animal intakes, manure production, and crop/animal emissions follows the Intergovernmental Panel on Climate Change's (IPCC) guidelines (IPCC 2006c). This is supplemented with the establishment of animal metabolism balances. See section 4.1 in Merciai and Schmidt (2016) for more information.

The Energy Module

The energy module aims to rearrange the data included in the energy supply and use tables (En-SUTs) (Stadler et al. 2015) in a format that is suitable for being used in the MR-HSUTs. This is done in accordance with energy supply data from the IEA (2015).

En-SUTs follow an approach advised by official guidelines of international institutes (OECD et al. 2004). According to such guidelines, energy flows produced by waste activities are inserted in the energy activities. Further, combined heat and power plants (CHP plants) (Darrow et al. 2015;

EURELECTRIC 2014) are two separated activities, one producing only heat and one only electricity.

We have moved the production of electricity and biogas obtained from waste treatment from energy sectors to waste sectors. In this way, energy flows become by-products of waste activities (Nakamura and Kondo 2009; Schmidt et al. 2010). Furthermore, the CHP productions are aggregated into one activity, with heat as principal production and electricity as by-product. This is the default procedure. However, some of the CHP plants are so-called extraction plants, which can vary their production of electricity and heat independently. Technically, this is done by switching between back-pressure mode (fixed electricity to heat production) and condensation mode (only electricity production) (Darrow et al. 2015; EURELECTRIC 2014). Therefore, by following the kind-of-activity units (EC et al. 2008, 88–89), the extraction plants can be subdivided into CHP plants (back-pressure) and pure electricity production (condensation mode). The subdivision is made by assuming that CHP plants belong to heat production, and that they have a maximum electricity-to-heat ratio at 0.5 (elaborations of EURELECTRIC [2014] and Darrow et al. [2015]). Then, all remaining electricity is supplied by condensation mode in CHPs, and this is reclassified to belong to the electricity sector. See section 4.2 in Merciai and Schmidt (2016) for more details.

Technical Coefficient Module

This module is the first general module in figure 2 and fulfils several tasks. First, there is a revision of data, which also concerns fixing the gaps in the collected data. Then, these revised data are used for the calculation of physical technical coefficients. Data have been collected from international agencies (BGS 2014; EUROSTAT 2015; FAO Statistic Division 2015; IFA 2015; UN 2015; USGS 2015; World Steel Association 2010; WU 2014).

Data Revision

Initially, data are classified according to an index of reliability that is based on the reliability of the data source. Usually, all the data sets of international agencies are considered reliable, unless we noticed that, for some countries or for some specific products, the data coverage was poor. Data indicated as "not definitive" by the data source is also considered of poor quality. Data from United nations (UN) on industrial commodities (UN 2015) is not considered reliable because often the products are compiled in units different from mass, for example, items, square meters, etc., so the conversion into mass may be a source of error. Therefore, they undergo a revision.

Data revision is aimed to validate poor quality data and to estimate missing data. The revision is divided in five steps that are explained in the following. See section 4.3.1 in Merciai and Schmidt (2016) for more information.

A *reasonability check* aims to detect outliers in the time series of collected data and it was applied to FAOSTAT data (see the Supporting Information available on the Journal's website). Indeed, few unexpected values were noticed in some time series probably due to changes in the classification or/and approach over the years, or by simply misreported values. Therefore, we have built this step, specifically aimed to this data source. For the remaining data, we almost never had a complete time series to revise; therefore, this procedure was not implemented for other data.

A *gap-filling procedure* is aimed to construct time series when only few values were available. Linear interpolation and extrapolation has been used for this. This procedure has been used for waste treatment data,[4] because data coverage was very poor.

A *price-based data estimation* derives the missing physical flow from monetary productions and average prices. Average prices are obtained dividing a proxy of the world total monetary production by a proxy of the world total physical production because country prices are not available at this stage of the algorithm. Only those countries that have both monetary and physical values are taken into account in the calculation of the world production (see the Supporting Information on the Web).

A *linkage to specific material* is implemented for collected production flows that are either not considered reliable or completely missing, and whose production usually occurs within a short distance from the material production. This principle has been applied for determining the cement production, which is assumed to be proportional with availability of aggregates (sand and gravel), using default coefficients taken from Hafner and colleagues (2010) and Rejman-Burzyńska and colleagues (2010). The availability of a product in a country is here meant as the amount of materials that can be directly used by activities, and it is equal to production plus import and less exports.

The *general data estimation procedure* is a generalization of the *linkage to specific material procedure*. It is used for missing or unreliable data that have not been estimated in the above steps, such as textile and chemical products. It is an iterative procedure. The existing information is used to estimate missing data, such as total uses of activities, imports, and exports for each country. This new estimated data, together with the already existing information, will be then used to estimate production data. After that, the procedure restarts until it is supposed to have reached a reasonable estimate (see the Supporting Information on the Web).

The underlying logic is that the volume of a specific product carried out by an activity depends on the amount of materials that enter into the activity, that is, the activity availability of materials, and that are converted into products. Available materials, which may be products, natural resources, or waste flows, are converted into products using default transformation coefficients taken from Schmidt (2010) and from LCA databases (www.ecoinvent.com).[5]

The transformation coefficients are activity specific and indicate the fraction of material that is embodied in the product output (Nakamura et al. 2007; Schmidt et al. 2012). We define a material that is embodied into a product as *feedstock material*.[6] The feedstock material may be also a portion of the total product used by an activity. For example, natural gas entering into

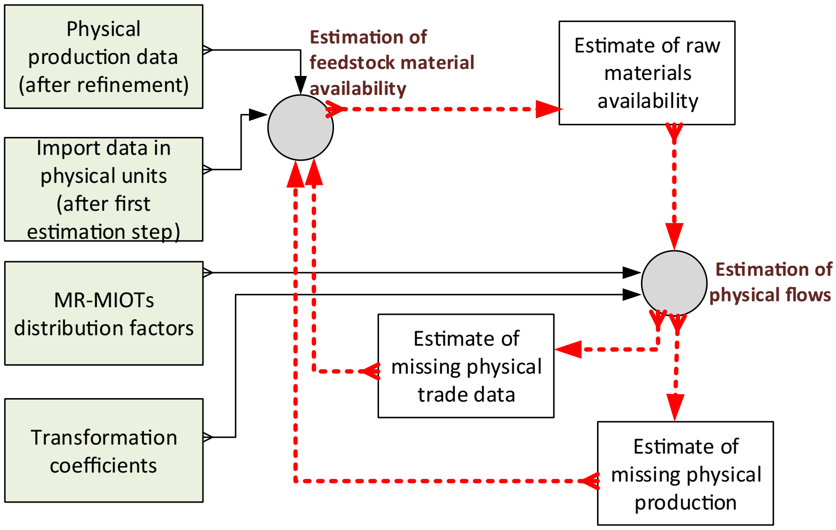

Figure 3 The iterative data generation procedure for the assessment of missing physical production. Dotted arrows show the flow of new data flows estimated in the iterative steps. Green boxes show collected data used by the procedure. White boxes indicate the estimated data. Gray circles indicate calculations. MR-MIOTs = multiregional monetary input-output tables.

plastic activities can be, in part, a feedstock material and, in part, combusted to produce heat. In the latter case, the material is defined as *combusted material*.

The activity availability of materials is determined distributing the total country availability of products. The distribution factors are derived from the relevant monetary product by product IOT (multiregional IOT). The procedure is illustrated in figure 3.

Technical Coefficients

To this point of the procedure, we have all the data to calculate physical technical coefficients, which are important for shaping the constraints in the next modules of the algorithm. The physical technical coefficients that are calculated are the (*product*) *input coefficients* and *by-product coefficients*. The former indicates how much of an input feeds to an activity per unit of principal production, while the latter indicates how much of secondary production is provided per unit of principal production. For secondary production, we consider only by-products technologically linked to the principal production (EC et al. 2008; 514, def. 28.46.b and def. 28.46.c). *By-product coefficients* are derived from sectorial modules or from literature (e.g., www.ecoinvent.org, Merciai and colleagues [2013], and Schmidt [2010]). *The by-product coefficients* $(\mathbf{C})$ are then used to split the total national production $(\boldsymbol{v})$ in principal $(\boldsymbol{v}_{princ})$ and secondary $(\boldsymbol{v}_{by-prod})$ as in equation (1).

For simplifying the formulations in the text, we assume a squared framework meaning that the SUTs are square (equation 1).

$$\begin{aligned} \boldsymbol{v}_{princ} &= (\mathbf{C}+\boldsymbol{I})^{-1} \times \boldsymbol{v} \\ \boldsymbol{v}_{by-prod} &= \boldsymbol{v} - \boldsymbol{v}_{princ} \end{aligned} \tag{1}$$

As a consequence of equation (1), the supply table $(\mathbf{V}'_{\mathrm{T}})$ can be constructed taking into account off-diagonal productions (see equation 2).

$$\mathbf{V}'_{T} = (\mathbf{C}+\boldsymbol{I}) \cdot \boldsymbol{diag}(\boldsymbol{v}_{princ}) \tag{2}$$

Input coefficients $(\mathbf{A})$ are obtained distributing available materials over the activities (see equation 3):

$$\mathbf{A} = \boldsymbol{diag}\left[\boldsymbol{v} + \breve{\boldsymbol{m}}_{T} - \breve{\boldsymbol{e}}_{T}\right] \cdot \boldsymbol{U}_{distr} \cdot \boldsymbol{diag}(\boldsymbol{v}_{princ})^{-1} \tag{3}$$

where $\mathbf{U}_{\mathrm{distr}}$ shows the partition of the total national consumption over the activities, and $\breve{\mathbf{m}}_{\mathrm{T}}$ and $\breve{\mathbf{e}}_{\mathrm{T}}$ are the initial vectors of imports and exports, respectively. The calculation of $\mathbf{A}$ is done for each geographical region.

Input coefficients $(\mathbf{A})$ also undergo sanity checks to verify their validity. In practice, high values are replaced whenever they are bigger than a defined upper limit. With this aim, values of country-specific matrices $\mathbf{A}$ are used to construct normal distributions (Bain and Engelhardt 2000) for each input entering into one activity. Afterward, values higher than 2 times the standard deviation (σ) plus the mean (μ) are replaced with an amount equal to this upper limit.

Trade Module

The idea is that, keeping the collected data on supply of products constant, each country needs a certain amount of feedstock to justify production, for example, to produce 1 kg of paper, a certain amount of pulpwood is needed. Available feedstock can be produced domestically or imported. We define as *minimum material requirement* $(\boldsymbol{f}_{MMR})$ the lower limit of the country availability of products. $\boldsymbol{f}_{MMR}$ is calculated multiplying the coefficient matrix by the vector of principal productions plus a proxy of the products consumed by final demand. The physical trade module does not change the monetary trade flows. For simplicity, from now on we avoid using the suffix T that indicates the hybrid units.

Before performing the trade balance, two types of data conflicts are addressed:

a. A country needs to import a certain quantity of a material, but the exporting countries do not export enough. Solved by adding import from other countries, selected among major exporters;
b. A country does not produce and import enough to satisfy its requirement. Solved by adding import from other countries, selected among major exporters.

The balancing procedure consists of an entropy optimization problem. The logic behind is that the material available in one economy may come from domestic production and import. A deficiency of material may be resolved with more imports or reducing the overall demand of that product. The latter is implemented either assuming that the activities asking for that material may increase their internal use to reduce the overall country request or increasing purchaser price. Internal use is allowed only for activities whose productions have a lower reliability. Therefore, this mechanism can be seen as an ultimate revision of production data.

The following constraints translate this idea in formulas. For clarity's sake, let us assume that the supply $(\mathbf{V})$ and use table $(\mathbf{U})$ is square. i indicates a product, while j indicates an activity. A generic element (i,i) indicates a value on the main diagonal. h replaces i and j (equations 4 through 10).

$$\boldsymbol{m_i - e_i + V_{i,i} - U_{ii} + \sum_{j \neq i} V_{i,\,j} \geq f_{\mathrm{MMR},i} - \hat{u}_i} \quad \forall \ \textit{product i and} \ \forall \ \textit{country c} \tag{4}$$

$$\boldsymbol{\hat{u}_i \leq \sum_{h \neq i} (U_{h,h} * \tilde{A}_{ih}) + \sum_{k \neq i} [(1 - \Delta p_{i,k}) * V_{k,k} * \tilde{A}_{ik}]} \quad \forall \ \textit{product i and} \ \forall \ \textit{country c} \tag{5}$$

$$\boldsymbol{m_i = i' \cdot N_i\,(.,c)} \quad \forall \ \textit{product i and} \ \forall \ \textit{country c} \tag{6}$$

$$\boldsymbol{e_i = N_i\ (c,.) \cdot i} \quad \forall \ \textit{product i and} \ \forall \ \textit{country c} \tag{7}$$

$$\boldsymbol{V_{i,i} + \sum_{j \neq i} V_{i,\,j} > e_i} \quad \forall \ \textit{product i and} \ \forall \ \textit{country c} \tag{8}$$

$$\boldsymbol{\sum_c e_i^c = \sum_c m_i^c} \quad \forall \ \textit{product i} \tag{9}$$

$$\boldsymbol{U_{i,i} < V_{i,i} * k_i} \quad \forall \ \textit{product i and} \ \forall \ \textit{country c} \tag{10}$$

Equation (4) states that the available material must be higher than the minimum material requirement $(\mathbf{f}_{\mathrm{MMR,i}})$. The material available on a national market may come from the net trade $(\boldsymbol{m_i - e_i})$ and from the domestic production $(\mathbf{V}_{\mathrm{i,i}} - \boldsymbol{U_{ii}} + \sum_{\mathrm{j \neq i}} \mathbf{V}_{\mathrm{i,j}})$, where $\mathbf{V}_{\mathrm{i,i}}$ is the principal production, $\boldsymbol{U_{ii}}$ the increased internal use,[7] and $\sum_{\mathrm{j \neq i}} \mathbf{V}_{\mathrm{i,j}}$ the off-diagonal production. On the right side, the minimum material requirement of product i $(\mathbf{f}_{\mathrm{MMR,i}})$ may be reduced if there is a decrease of its indirect request by other activities $(\hat{\mathbf{u}}_{\mathrm{i}})$. The latter quantity is described in equation (5). The first part on the right hand indicates a reduction of the demand for product i when used as feedstock material. $\tilde{\mathbf{A}}_{\mathrm{ih}}$ is a special matrix of coefficients that includes only feedstock materials. The second part shows a reduction of the request for non-feedstock product i. $\tilde{\mathbf{A}}_{\mathrm{i,k}}$ is a coefficients matrix that excludes feedstock materials while $\Delta\mathbf{p}_{\mathrm{i,k}}$ indicates the distance of the price paid by activity k to purchase i respect to the default average price of i $(\overline{\mathbf{p}}i)$. The fluctuation of prices is constrained.

Equations (6) and (7) show the national balance of imports and exports. $\mathbf{N}$ is the three-dimensional physical trade matrix ($\mathrm{country_{importer}XproductXcountry_{exporter}}$). $\mathbf{N}_{\mathrm{i}}(.,\mathrm{c})$ and $\mathbf{N}_{\mathrm{i}}(\mathrm{c},.)$ indicate the imports and exports of country c of product i respectively. It is assumed that a country cannot export more than what it produces (equation 8). This is aimed to limit the re-exports. Equation 9 indicates the world trade balance. Equation 10 shows that internal uses have an upper limit as a fraction of total production $(\mathbf{k}_{\mathrm{i}})$, by default set to 10%.

Equation (11) shows the optimization function (OF), which minimizes a cross-entropy function:

$$\boldsymbol{OF} = \min \left\{ \sum_{i,c',c''} \mathbf{N}_i(\boldsymbol{c}', c'') \cdot \left(\log \left(\mathbf{N}_i(\boldsymbol{c}', c'') \middle/ \check{\mathbf{N}}_i(\boldsymbol{c}', c'') \right) \right) \right\} \tag{11}$$

where $\mathbf{N}_{\mathrm{i}}(\mathbf{c}'\mathrm{c}'')$ is the final estimate trade flow between exporting country c' and importing country c'' of product i, while $\check{\mathbf{N}}(\mathbf{c}'\mathrm{c}'')$ is the initial estimate.

Balancing Module

The modules presented so far have contributed to determine the necessary information to build national hybrid supply and use tables (HSUTs). This information is then used to generate initial estimates of the SUTs. The balancing module aims to balance these initial estimates. The procedure is implemented for each country.

Balanced tables means that, first, the total supply and use of any product must be equal. Then, we impose a mass and energy balance within each activity. With regard to the mass balance, the mass of incoming products is either embodied in the supplied products, emitted, discharged as waste, or accumulated in the economy (stock addition). With regard to energy balance, we assure that the energy the energy input relative to output is within a defined range. We use efficiency factors for this (EURELECTRIC 2003). We do not publish emissions of heat or other loss of energy. Mass balances are implemented for activities whose principal production is accounted in mass units, and likewise energy balances.

An optimization problem is constructed for balancing country HSUTs, subjected to the constraints in equations (12) to

(16). The following matrices and vectors are in mixed units. For simplicity, the suffix (T) is not shown.

$$\boldsymbol{U} \cdot \boldsymbol{i} + \boldsymbol{FD} \cdot \boldsymbol{i} + \boldsymbol{e} \ = \mathbf{V}' \cdot \boldsymbol{i} + \boldsymbol{m} \tag{12}$$

$$\boldsymbol{dm}' \cdot [(\boldsymbol{U} - \boldsymbol{U}_{\boldsymbol{comb}}) * \boldsymbol{D}] + \boldsymbol{dm}_{\boldsymbol{R}}' \cdot (\boldsymbol{R} * \boldsymbol{F}) + \boldsymbol{dm}_{\boldsymbol{W}}' \cdot (\mathbf{W}_{\boldsymbol{U}} * \boldsymbol{T}) = \boldsymbol{dm}' \cdot (\mathbf{V}') \tag{13}$$

$$\boldsymbol{U} \geq \boldsymbol{U}_{\boldsymbol{comb}} \tag{14}$$

$$\boldsymbol{V}_{\boldsymbol{X}} \cdot \boldsymbol{i} \geq \left[(\boldsymbol{U}_{\boldsymbol{comb}}(.;\boldsymbol{x})' * \boldsymbol{U}'_{\boldsymbol{X}}) \cdot \boldsymbol{cv} \right] * \boldsymbol{eff}_{\boldsymbol{X}} \tag{15}$$

$$\boldsymbol{D}_{\boldsymbol{low}} \leq \boldsymbol{D} \leq \boldsymbol{min}(\boldsymbol{D}_{\boldsymbol{up}} | \boldsymbol{B}_{\boldsymbol{Use}}) \tag{16}$$

Equation (12) assures that supply and use of products are balanced. On the left side, $\boldsymbol{U}$, $\boldsymbol{FD}$, and $\boldsymbol{e}$ are, respectively, the use matrix, the matrix of final demand, and the vector of export. On the right side, **V'** and $\boldsymbol{m}$ are the supply matrix and the vector of import, respectively. $\boldsymbol{i}$ indicate generic summation vectors.

Equation (13) establishes the mass balance within activities. $\boldsymbol{U}_{\boldsymbol{comb}}$, $\mathbf{R}$, and $\mathbf{W}_{\mathbf{U}}$ are the matrix of combusted materials, matrix of natural resources, and, finally, the use of waste matrix. $(\mathbf{U} - \mathbf{U}_{\mathrm{comb}})$ indicates that only feedstock materials can be embodied in the produced output. $\boldsymbol{dm}$ indicates the DM vectors of the various inputs (Merciai et al. 2013, Table 6.1). $\boldsymbol{D}$, $\boldsymbol{F}$, and $\boldsymbol{T}$ are the transformation coefficients for goods, resources, and waste fractions, respectively. These values are calibrated using the same default values used for EXIOBASE v2 (Merciai et al. 2013, see 6.1)

Equation (14) assures that an input of materials cannot be lower than combusted materials. The matrix of combusted material is determined in the energy module and is kept constant. Equation (15) shows the energy balance for processes delivering intangible energy products, that is, electricity and heat, as principal production (the subscripted x indicates these activities). In Equation (15), the output of activities in energy units, that is, $\mathbf{V}_{\mathrm{X}} \cdot \mathbf{i}$, has an upper limit equal to the maximum process efficiency $(\boldsymbol{eff}_{\boldsymbol{x}})$ (EURELECTRIC 2003) times the energy input $(\mathbf{U}'_{\mathrm{comb}}(.;\mathbf{x}) * \mathbf{U}'_{\mathrm{X}})$. $\mathbf{U}'_{\mathrm{X}}$ is used to select only the energy flows that are combusted in order to produce principal productions.[8] $\mathbf{cv}$ is a vector of calorific values that is used to convert mass of inputs into energy.

Equation (16) defines that a transformation coefficient has a predefined lower limit $(\mathbf{D}_{\mathrm{low}})$ and upper limit $(\mathbf{D}_{\mathrm{up}})$ (Schmidt 2010), which takes into account that an input may be emitted according to exogenous emission factors $(\mathbf{B}_{\mathrm{use}})$ (Stadler et al. 2015). These emissions factors will be used later in the algorithm to determine the emission accounts.

The optimization function (OF) of the balancing optimization problem is an entropy function:

$$\boldsymbol{OF} = \min \left\{ \sum_{i,j} \left(\boldsymbol{U}(\boldsymbol{i},\ \boldsymbol{j}) \cdot \log \left(\boldsymbol{U}(\boldsymbol{i},\ \boldsymbol{j}) \middle/ \check{\boldsymbol{U}}(\boldsymbol{i},\ \boldsymbol{j}) \right) \right) \right\} \tag{17}$$

where $\boldsymbol{U}(\boldsymbol{i},\ \boldsymbol{j})$ is the final use of material i by activity j and $\check{\boldsymbol{U}}(\boldsymbol{i},\ \boldsymbol{j})$ is the initial estimate.

In the balancing procedure, the supply of products (**V'**), the trade, the DM coefficients, the inputs of combusted materials, the efficiency of energy processes, and some special inputs determined in sectorial module (e.g., input of fertilizers or animal feed intake), are all kept constant. This means that most of the uses in matrix **U** and the product transfer coefficients (**D**) are the only variables determined by the procedure. The use and supply of waste treatment services are not calculated at this stage, but will be done when waste accounts are defined (see Section *Waste Accounts and Stock Addition*).

In general, besides the change of inventories, all the values must be non-negative. Once this crucial module is performed, the next steps consist of merging all the national HSUTs in a multiregional format and, finally, calculating the extensions.

Final Module

In this module, all the national tables are combined together using the information of the physical trade matrix. By doing that, all the transactions within and between countries are determined. Afterward, the extensions are calculated so that the MR-HSUTs are finally completed. In the following, these steps are described more in depth.

The table of multiregional transactions are constructed combining national tables and the trade matrices.

Auxiliary Accounts

Once the national and international transactions are built, the algorithm determines auxiliary accounts that are:

a. Supply/use of waste fractions from packaging;
b. Supply/use of waste fractions from vehicles;
c. Supply/use of waste fractions as a consequence of trade of heterogeneous products;
d. Supply/use of crop residues, energy crops, and grass.

The first accounts are necessary to trace the path of packaging coming with products. The second and third accounts are necessary to have a breakdown into homogenous waste fractions of products made of many different materials (b and c). These accounts are calculated considering the trade between countries. Finally, the fourth gives information on the supply and use of crop residues, energy crops, and grass eaten by animals. These accounts are defined as auxiliary because they provide extra information that is not directly used for the mass balance of activities (equation 13), but it is nevertheless important for determining waste accounts. Only crop residues, which may be considered as by-products of agriculture without market price, are taken into account in the mass balance procedure.

Waste Accounts and Stock Addition

The waste accounts show the supply and use of waste fractions by activities. The approach here applied shares the same principles of (Nakamura and Kondo 2009; Schmidt et al. 2010), although the way to calculate some supply flows differ (see *Discussion* section).

The use of waste, which is the quantity of waste materials handled by waste treatment activities, is easily calculated. The supply of waste treatment services, as described above, is obtained from data collection or estimated. Therefore, the use of waste is obtained multiplying this supply by conversion factors, which link waste treatment services (e.g., recycling or incineration) to waste fractions (paper, glass, etc.). Due to the high detail of the waste activities' classification, the conversion factors are obtained quite straightforwardly.

The supply of waste materials is calculated based on mass balance. Initially, for each activity, the *potential supply of waste* is calculated, which includes all the inputs that are neither embodied in the supply of products nor emissions. An input may be a product, a natural resource, or waste. The potential supply of waste is then divided into *ordinary waste* and *stock addition*. Ordinary waste is the waste discharged in the same period (year) of the "purchase," while the stock addition consists of products accumulated at the end of the period. For each waste fraction, the following balance is performed:

$$\begin{aligned} &\textit{use of waste} + \textit{unregistered waste} \\ &\quad = \textit{suply of ordinary waste} + \textit{reduction of accumulated materials} \end{aligned}$$

If the use of waste is higher than the supply of ordinary waste, it is assumed that materials accumulated in previous periods are discharged. Contrarily, it is assumed that there is some unregistered waste if the calculated supply of waste is higher than the collected data on the use of waste (treatment).

Once the supply of waste by activities is calculated, the demand of waste treatment services, which is part of the use matrix, can be determined by multiplying the production of waste fractions by partition factors. Partition factors, which are country specific and based on the supply of waste treatment services, tells how much of a fraction is handled by the different waste treatment services in each country. For example, a partition factor says how much paper is handled by recycling, landfilling, incineration, and composting.

Emissions and Resources Accounts

Some emissions have been calculated in the sectorial modules, such as the agricultural module. The remaining are calculated by use of emission factors multiplied with physical flows (Stadler et al. 2015; Merciai and Schmidt 2016). Calculated emissions are related to:

a. combustion of fossil fuels and renewables;
b. waste treatment;
c. supply of products (process emissions);
d. agricultural activities (this is described in the agricultural module);
e. the use of products (e.g., use of chemicals);
f. unregistered waste;
g. avoided emissions (see footnote 3).

Emissions from combustion, waste treatment, and related to the supply and use of products are obtained by multiplying the combusted materials, treated waste fractions, and supplied/used products with emission factors (Stadler et al. 2015). The emissions from unregistered waste take into account the carbon dioxide (CO_2) from decomposition of the waste materials. Emissions a to e are aggregated, while emissions f and g are inserted as a separate account.[9]

Resources of extracted materials are derived directly from the supply of specific sectors, such as crop cultivation and mining activities or extraction of crude oil (Stadler et al. 2015), by using transfer coefficients, that is, $\boldsymbol{F}$. Resources extracted by crop cultivation are derived by using data on main contents of fat, calories, proteins, etc. (Gebhardt and Thomas 2002) converted into substances (Munoz et al. 2008). Oxygen for fuel combustion and animal and human respiration is based on mass balances of combustion and animals/humans (Schmidt 2010).

Results

This section shows life cycle greenhouse gases (GHGs) emissions results for selected product categories, and comparisons are made with other life cycle databases. The aim is to have a quick sanity check of the macro and micro results obtained with EXIOBASE. We start with macro results, where we will analyze the performances of countries. Then, we will move toward micro analyses, where product footprint will be compared.

Figure 4 shows the territorial GHG emissions of the EXIOBASE countries/regions. The territorial emissions are divided into activities (orange bar) and final consumers (blue bar). These emissions are compared to the results obtained by the EDGAR data set (PBL 2017) (blue line).

The comparison in figure 4 reveals that most countries show lower values for EDGAR, while a few countries, such as Greece, Denmark, Cyprus, Malta, and South Africa, have higher values. On the global scale, EDGAR shows 10% higher GHG emissions than EXIOBASE. The reasons for this are: EXIOBASE does not include land-use change emissions, while EDGAR does; EXIOBASE redistributes the emissions from international aviation and bunkers (Stadler et al. 2015), while EDGAR does not; here we account only CO_2, nitrous dioxide and methane while EDGAR also includes F-gasses. Further, differences in emission models and related input parameters may explain the difference between EXIOBASE and EDGAR emissions.

The second series of results regard micro analyses, that is, product carbon footprints. The aim is to illustrating that EXIOBASE can also be used for product-based analysis, such as life cycle assessment. For that aim, two product groups in EXIOBASE have been compared with corresponding products in the ecoinvent Database v3.2 (ecoinvent Center 2017). The

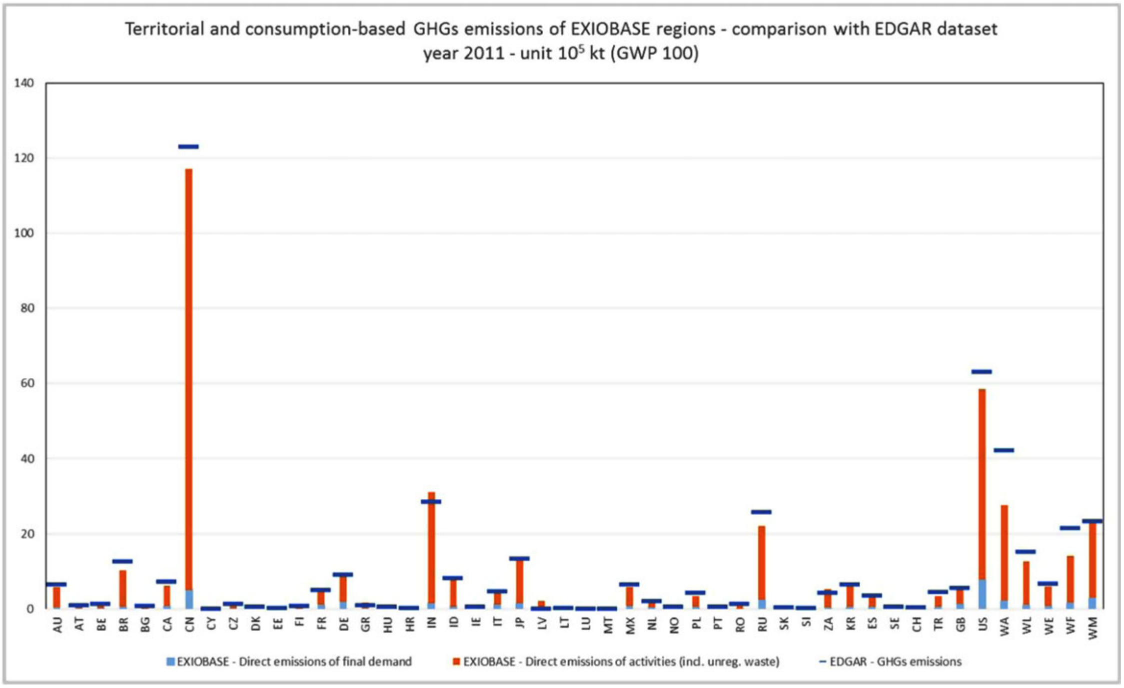

Figure 4 Territorial GHGs emissions of the EXIOBASE regions. Territorial emissions (bars) are divided into activities (orange bar) and final consumers (blue bar). The blue line shows the national GHGs emissions as retrieved from EDGAR data set. GHGs = greenhouse gases; GWP100 = global warming potential for a 100-year time horizon; kt CO_2-eq = kilotonnes of carbon dioxide equivalent.

comparison is presened for two product groups: dairy and aluminium products. These products are chosen because the product classification in EXIOBASE and ecoinvent are relatively similar. We have chosen the consequential system model in ecoinvent because the Stone's method is applied in EXIOBASE for the calculations. Global product average from ecoinvent was used. It has been noted that with EXIOBASE, there are no cutoffs as instead occurs in ecoinvent (Majeau-Bettez et al. 2011).

Figure 5 shows the carbon footprint per kg of DM dairy products in EXIOBASE. The dairy product group includes different products, such as milk, cheese, yogurt, powder, etc., that are different from country to country. The EXIOBASE carbon footprints in figure 5 are compared with two dairy products from ecoinvent, namely cheese and yogurt. The following ecoinvent data sets were used "Cheese, from cow milk, fresh, unripened{GLO}| market for | Conseq" and "Yogurt, from cow milk {GLO}| market for | Conseq." It is assumed that yogurt and cheese have DM at 12% and 50%, respectively (based on Gebhardt and Thomas [2002]).

Figure 5 shows that, in most countries, the carbon footprint of dairy products in EXIOBASE are within the carbon footprint of the two ecoinvent dairy products. The differences in results are mainly related to differences in modeling, such as substitution caused by beef by-product in the cow milk production (beef in EXIOBASE and sheep in ecoinvent), cutoffs, different models for methane emissions from enteric fermentation, different losses throughout the product chain, different electricity mixes, and, further, ecoinvent includes some land-use change emissions, which are not included in EXIOBASE. Some countries show outliers (India and Malta), which may be explained with uncertainties in statistical input data.

The second product analysis regards the aluminium production (see figure 6). We have selected the ecoinvent v3.2 process "Aluminium, primary, liquid {GLO}|Market for | Conseq" as upper limit and the process "Aluminium, primary, ingot {IAI Area, EU27 & EFTA}|Market for | Conseq" as lower limit. As for the dairy case, it can be seen that the the EXIOBASE results fall into the interval for most countries. Some of the difference between countries can be explained by difference in carbon footprint for the electricity, that is, countries with a high share of coal and natural gas as sources of electricity tend to have high aluminium footprints.

Discussion

It is demonstrated that the EXIOBASE multiregional hybrid IOTs (MR-HIOTs) are founded in economy-wide detailed economic, mass, and energy balance, and that it can have multiple applications from micro to macro scale (Schmidt and Merciai 2014; Tisserant et al. 2017; Usubiaga et al. 2017; Wood et al. 2015, 2017). Our ambition is to create a data set that can be used for country, sector, and product group-specific analyses. Such a model can serve as a common multipurpose tool, or at least a common starting point for analysis that may create a stronger bound between I-O, industrial ecology, and ecological economy communities (Pauliuk et al. 2015; Suh and Kagawa 2005; Tukker et al. Forthcoming). The MR-IOTs published so

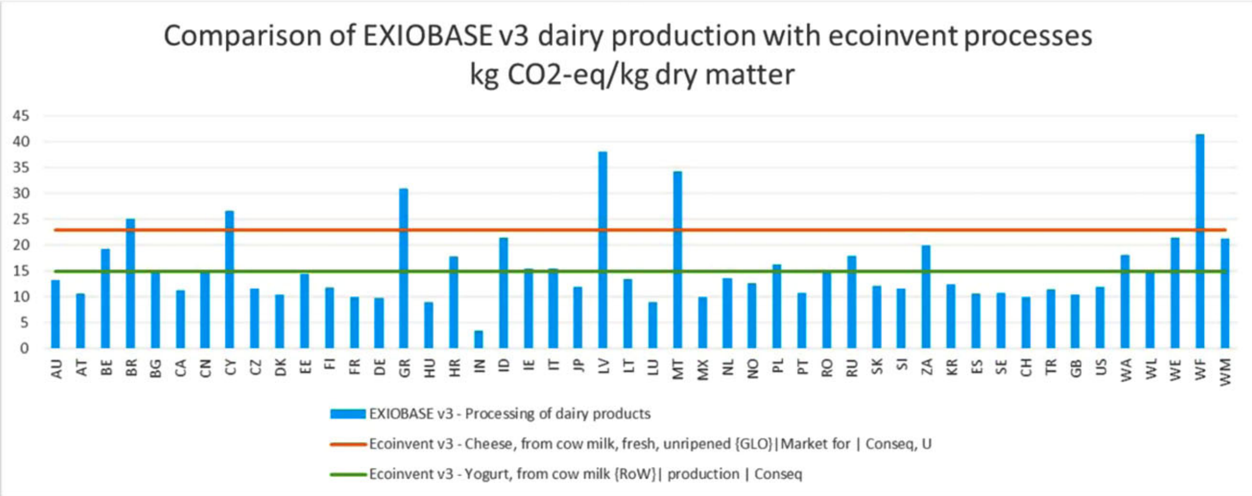

Figure 5 Carbon footprint of dairy product in EXIOBASE and for two selected dairy products in ecoinvent v3.2. kg CO_2-eq/kg = kilograms of carbon dioxide equivalent per kilogram.

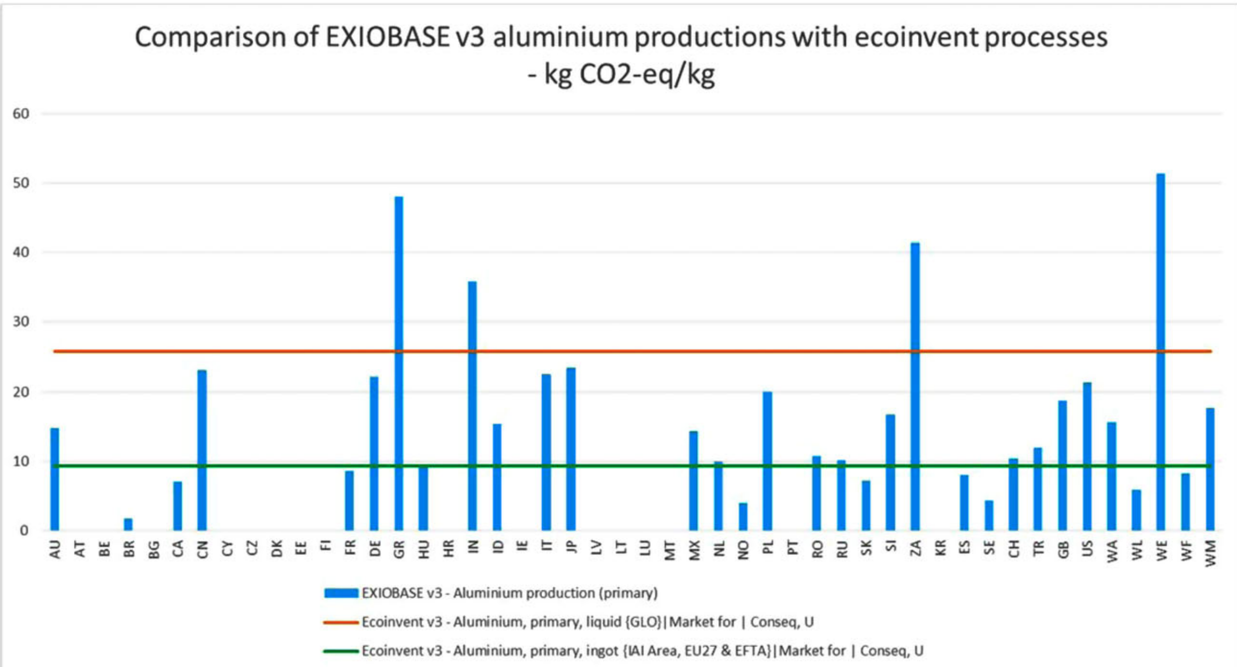

Figure 6 Carbon footprint of aluminium products in EXIOBASE and for two selected products in ecoinvent v3.2. kg CO_2-eq/kg = kilograms of carbon dioxide equivalent per kilogram.

far are all expressed in monetary units, which often makes it difficult to link to tangible flows and policy targets. For example, the detailed waste module accomplished with physical waste flows and their treatments facilitates a direct link to several policy targets on, for example, circular economy.

Obviously, the multilayer balance approach introduces more computational complexity compared to monetary models. Contrarily, the monetary models lack general consistency in terms of other balances than economic flows (Majeau-Bettez et al. 2016; Merciai and Heijungs 2014), and further basic physical requirements to production functions are not checked, for example, that sufficient feedstock materials are available to justify production. In other words, monetary tables may bear an uncertainty that is hard to quantify. However, EXIOBASE is limited to three balanced levels, which means that balances in other levels, such as individual substances and water, are yet to be addressed in the future.

MR-HSUTs can be considered as an attempt of harmonizing many segmented data sets. While a great work of homogenization of economic statistics has been initiated in the latest decades producing reliable data sets, the corresponding physical flows are still only partially covered or documented with data of varying quality. We have encountered several challenges due to data shortage, therefore correcting and compensating procedures have been introduced. In many cases, we have adopted simple methodologies, mainly due to the shortage of time in the DESIRE project. In the future, we aim to improve the algorithm, for example, internalizing the advancements that occurred in the literature, such as the advanced cross-entropy approaches (Többen 2017, Caggiani et al. 2014; Rodrigues 2014; Lenzen et al. 2009), performing sensitivity and inferential analyses, and adding more unit levels.

Another feature of EXIOBASE, which makes it different from other MR-HIOTs, is the waste module that includes a detailed accounting for the supply and use of waste throughout the economy. The applied approach in EXIOBASE was developed through the FORWAST project (http://forwast.brgm.fr) and highly inspired by the waste input-output model introduced by Nakamura and Kondo (2002). We have used the concept of the matrix $\boldsymbol{S}$ (Nakamura and Kondo 2002, 44–46), which converts the supplied flows of waste fractions (our supply of waste accounts) into demand of waste treatment services (accounted in the matrix of transactions). The economy-wide balance balances in EXIOBASE enables calculating waste flows and comparing the calculated supply of waste with national waste statistics. The difference between the calculated supply of waste and the data collected on waste treatment is regarded as "unregistered waste" and emissions related to its decomposition are also accounted. This quantity is endogenously determined by the algorithm. Therefore, the matrix $\boldsymbol{S}$, which is shaped by official statistics, is generalized introducing the possibility of incomplete statistics that, for example, could be caused by illegal dumping. Another common approach is the use of transfer coefficients introduced by Nakamura and colleagues (2007, 54), which are included in the matrices $\boldsymbol{D}$, $\boldsymbol{F}$, and $\boldsymbol{T}$.

Conclusions

It has been described how the MR-HSUTs are calculated for EXIOBASE v3. These are the first global multiregional tables in hybrid units ever published. The advantages of the hybrid structure include several dimensions of balance checks, which give more robustness to the data set (Ayres 1995), and the ability to operate with different prices per purchaser (when using physical mass or energy unit), which avoids miscalculations of impact accounted in mass units (Merciai and Heijungs 2014). An activity-based classification has been adopted, as opposed to industry-based classification commonly used. This makes the MR-HSUTs more process-based oriented, therefore the link to life cycle assessment is straightforward. Besides the above-mentioned properties of the model, the procedure for producing MR-HSUTs has been highly automated, which eases updates and error fixing. The limitations of the approach lie in the rather intensive data dependency and, for some parts of the data set, in the strong adoption of assumptions due to data shortage.

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Notes

1. We have also performed a monetary balance once the hybrid tables were constructed assuming different prices per purchaser. However, here in the text we exclude this part.
2. There is a major lack of statistical data for Taiwan (Taipei City) and it is not included as a separate country in the MR-HSUTs.
3. To avoid unbalances due to the different composition of fertilizer and manure, given the same amount of nutrients, a procedure following consequential life cycle assessment principles (Dalgaard et al. 2014) is applied. This procedure implies that the avoided emissions due to the application of manure, which substitutes chemical fertilizers, are taken into account in the manure treatment activity.
4. See table 2.9, in Merciai and colleagues (2013) for a list of references on waste flows.
5. This procedure cannot be applied to activities extracting raw material, such as mining activities, because in this case feedstock materials are natural resources. Therefore, all the missing mining products were determined in previous steps.
6. Feedstock materials are indicated as *primary inputs* by Nakamura and colleagues (2007).
7. U_{ii} is initially set to zero.
8. $\mathbf{U}'_{\mathrm{X}}$ is inserted so that, for example, fuels used for transportation are not taken into account.
9. In the delivered version, avoided emissions are inserted in the agricultural emissions, with a negative sign, but are also inserted separately for transparency.

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Supporting Information

Supporting information is linked to this article on the *JIE* website:

Supporting Information S1: This supporting information provides details on a procedure for detecting outliers, notes on the use of world average prices, and explanation of a general data estimation procedure.