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published in
Science of the Total Environment
2019

DOI (link to publisher)
10.1016/j.scitotenv.2018.12.194

document version
Publisher's PDF, also known as Version of record

document license
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Science of the Total Environment 658 (2019) 768–776

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

A tool to guide the selection of impact categories for LCA studies by using the representativeness index

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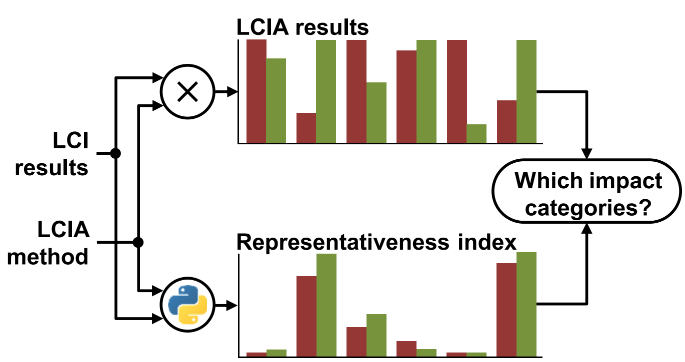
HIGHLIGHTS

- Representativeness index (RI) contextualizes the LCA results of each LCI result.
- An operational tool to compute RI is proposed (python package).
- An orthogonalization procedure is defined to solve impact correlation issue.
- RI tendencies of the whole ecoinvent database are discussed.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 12 April 2018
Received in revised form 12 December 2018
Accepted 12 December 2018
Available online 17 December 2018

Editor: D. Barcelo

Keywords:
LCA
Life Cycle Inventory
Life Cycle Impact Assessment
Representativeness
Dimension reduction
Interpretation tools

ABSTRACT

Understanding the environmental profile of a product computed from the Life Cycle Assessment (LCA) framework is sometimes challenging due to the high number of environmental indicators involved. The objective here, in guiding interpretation of LCA results, is to highlight the importance of each impact category for each product alternative studied. For a given product, the proposed methodology identifies the impact categories that are worth focusing on, relatively to a whole set of products from the same cumulated database.
The approach extends the analysis of Representativeness Indices (RI) developed by Esnouf et al. (2018). It proposes a new operational tool for calculating RIs at the level of impact categories for a Life Cycle Inventory (LCI) result. Impact categories and LCI results are defined as vectors within a standardized vector space and a procedure is proposed to treat issues coming from the correlation of impact category vectors belonging to the same Life Cycle Impact Assessment (LCIA) method. From the cumulated ecoinvent database, LCI results of the Chinese and the German electricity mixes illustrate the method. Relevant impact categories of the EU-standardized ILCD method are then identified. RI results from all products of a cumulated LCI database were therefore analysed to assess the main tendencies of the impact categories of the ILCD method. This operational approach can then significantly contribute to the interpretation of the LCA results by pointing to the specificities of the inventories analysed and for identifying the main representative impact categories.

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https://doi.org/10.1016/j.scitotenv.2018.12.194
0048-9697/

1. Introduction

While the main goal of the Life Cycle Assessment (LCA) framework is to quantify and assess all the potential environmental impacts of human activities (ISO, 2006), the study of results over a too wide range of environmental impacts can become inefficient and lead to unclear conclusions (Steinmann et al., 2016). To obtain those environmental impact results, the LCA framework is structured in four phases where the Life Cycle Inventory (LCI) phase is one of the key one; it describes a product, a process or an activity throughout its value chain and quantifies its system-wide emissions and resource extractions. An LCI database (of which ecoinvent (Wernet et al., 2016) is a prime example) contains a large number of unit processes, each of which specifies the inputs and outputs (such as electricity, plastic, fossil resources and pollutants) of activities (such as rolling steel or driving a truck). Those LCI unit process databases allow LCA practitioners modelling the whole value chain of their study in reasonable time. The result of an LCI is a list of quantified emissions and resource extractions, collectively indicated as elementary flows, aggregated over all (up to thousands) unit processes that make up the system. In a cumulated LCI database, the entries are not the unit processes but rather the system-wide elementary flows, for each included product. From the LCI result, the Life Cycle Impact Assessment (LCIA) phase then translates these elementary flows in terms of environmental impacts. Different LCIA methods are available, often with a name, such as ReCiPe (Goedkoop et al., 2009), Traci (Bare, 2011) and ILCD (EC-JRC, 2010a). Each LCIA method consists of a number of environmental impact categories (such as global warming and ecotoxicity) and proposes Characterization Factors (CFs) to quantitatively link the elementary flows to these impact categories. There are often ten or more such impact categories within each LCIA method (EC-JRC, 2010b). Although aiming at being holistic, such large sets of impact categories can challenge the efficiency of environmental regulations (like product eco-design, decision making or environmental labelling). Further modelling the impacts into so-called endpoint damage levels could resolve the issue related to large sets. However, due to uncertainties, all models which are presently available are still classified as “interim” (Hauschild et al., 2013).

A reduction in the number of impact categories, by selecting the most relevant impact categories to focus on, would enable more effective environmental optimization. For comparative LCA, existing practices for normalization and weighting use external valuation of impact categories that might guide LCA practitioners on a reduced subset of LCIA results to interpret (Lautier et al., 2010). However, these procedures are increasingly discouraged (Prado-Lopez et al., 2014). By quantifying the uncertainties, exploration of the relative importance of impact categories through the magnitude of differences between LCIA results can produce promising tools for comparative LCA (Mendoza Beltran et al., 2018).

Some authors used Principal Component Analysis (PCA), combined with uncertainty analysis or multi-objective optimization (Mouron et al., 2006; Pozo et al., 2012) to deal with the large number of environmental indicators. Sometimes, PCA was also applied on LCIA results with technical indicators to reveal the relationships between those indicators (Basson and Petrie, 2007; Bava et al., 2014; Chen et al., 2015; De Saxcé et al., 2014).

Steinmann et al. (2016) applied PCA over a large range of products and LCIA methods (all the LCIA results of 135 impact categories for 976 products provided by ecoinvent) to select impact categories. In order to deal with impact category units and the wide orders of magnitude of LCIA results due to the high diversity of reference flows, they proposed to apply a product ranking. An alternative approach was a log-transformation on LCIA results prior to using a multi-linear regression (Steinmann et al., 2017). As comment to this last article, Heijungs (2017) noticed that the reference flow values of the studied LCIA results affect the outcomes of their work. He suggested standardizing the LCIA results by their energy footprint to be free of the default reference flow. This emphasizes the need to address data heterogeneity.

Other studies that apply multivariate statistical analysis or multilinear regression on LCIA results of products from ecoinvent focus on revealing correlation or alleged redundancies between impact categories (Huijbregts et al., 2006; Pascual-González et al., 2016, 2015; Steinmann et al., 2017). The objectives of these studies were to predict LCIA results from a reduced number of proxy impact categories. All these approaches work on the impact category results alone, and do not consider LCI information and its translation to impact categories.

By translating the elementary flows in terms of impact categories, LCIA can be considered to be a dimension reduction technique: LCIs are described by LCI results with more than a thousand variables (elementary flows) while LCIA results are a much smaller number of environmental indicators. The remaining dimensions, which all have an environmental meaning, may not all be necessary for dealing with the main environmental issues of the studied product. As the environment is disturbed and even damaged by such diverse substance emissions or resource utilizations from different human activities, all impact categories should be covered, but some of them may not be essential for the conclusion of one particular product, for instance, because they are strongly correlated with other impact categories.

The representativeness index (RI) was recently proposed by Esnouf et al., 2018 to provide a relative measure of the discriminating power of LCIA methods. The RI is meant to explore the relative relevance of each impact category belonging to a LCIA method for a specific product. It does not assess the relevance of the environmental model behind impact categories of the LCIA methods, but it is an aid to LCA practitioners, so they might focus on a reduced number of impact categories that best represent the elementary flows associated with a particular product. Moreover, by studying the links between the RI of an entire LCIA method and the RIs of its constituent impact categories, some issues have been raised on the correlation of the representativeness of impact categories (Esnouf et al. (2018).

The aim of this paper is to further develop the potential benefits of the RI methodology and to discuss representativeness issues regarding non-orthogonal (i.e. dependent) impact categories, and ways to solve such issues. We also developed an operational tool to calculate RIs as a downloadable Python package from an open access deposit.

The present paper is organized as follows: in Section 2, the standardization of the vector space where the LCA study takes place and the proximity relationship between an LCI vector and LCIA method subspaces (or impact category vectors) is briefly revisited as it is the same framework as that explained in Esnouf et al. (2018). The algorithm of orthogonalization of impact categories to avoid redundancy issues within a LCIA method is presented. The approach is illustrated and discussed in Section 3 on the ILCD method for two product results from the cumulated ecoinvent database (Wernet et al., 2016). Main tendencies of RI results over the cumulated LCI database are then explored. Finally, results from the decorrelation algorithm are analysed over the entire cumulated LCI database.

2. Material and method

Table 1 lists notations that are used in the present work. Vectors and matrices are distinguished from scalar by being written in bold, matrices are moreover capitalized.

2.1. RI methodology

2.1.1. Standardization and definition of an inner product

As proposed by several authors (Esnouf et al., 2018; Heijungs and Suh, 2002; Le Téno, 1999) the vector space where the LCA framework takes place is generated by a basis that represents the n elementary flows that are included in the study. The result of the LCI phase, for the ith product, can be described as a vector $\mathbf{g}_i$ (see Fig. 1.a). However,

Table 1
List of symbols and their meaning.

Symbol	Meaning
m	Number of products in LCI database
n	Number of elementary flows
p	Number of impact categories in a LCIA method
$\mathbf{g}_i$	LCI result vector of the ith product ($i = 1, \dots, m$)
$g_{x,\,i}$	The amount of the xth elementary flow for the ith product ($i = 1, \dots, m$; $x = 1, \dots, n$)
$\mathbf{q}_j$	The vector of characterization factors of the jth impact category: an impact category vector ($j = 1, \dots, p$)
$q_{x,\,j}$	The characterization factor of the jth impact category for the xth elementary flow ($j = 1, \dots, p$; $x = 1, \dots, n$)
$\mathbf{Q}$	LCIA method matrix composed of a set characterization vectors of p impact categories
$h_{j,\,i}$	LCIA result of the ith product on the jth impact category ($i = 1, \dots, m$; $j = 1, \dots, p$)
G_x	Geometric mean of $g_{x,\,i}$ for the xth elementary flow ($x = 1, \dots, n$)
$\tilde{\mathbf{g}}_i$	Standardized form of $\mathbf{g}_i$ (using the geometric mean) ($i = 1, \dots, m$)
$\tilde{\mathbf{q}}_j$	Standardized form of $\mathbf{q}_j$ (using the geometric mean) ($j = 1, \dots, p$)
$\tilde{\mathbf{Q}}$	LCIA method matrix consisting of standardized impact vectors $\tilde{\mathbf{q}}_j$
$\gamma_{j,\,i}$	Angle between $\tilde{\mathbf{q}}_j$ and $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m$; $j = 1, \dots, p$)
$\tilde{\mathbf{q}}_j^{\perp}$	Orthogonalized form of $\tilde{\mathbf{q}}_j$ (from a Gram-Schmidt process) ($j = 1, \dots, p$)
$\tilde{\mathbf{Q}}^{\perp}$	LCIA method matrix consisting of orthogonalized impact vectors $\tilde{\mathbf{q}}_j^{\perp}$
$RI_{j,\,i}$	Representativeness index of $\tilde{\mathbf{q}}_j$ for $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m$; $j = 1, \dots, p$)
RI_i	Representativeness index of LCI-result $\tilde{\mathbf{g}}_i$ for all impact categories ($i = 1, \dots, m$)
$RI_{j,\,i}^{\perp}$	Orthogonal representativeness index of $\tilde{\mathbf{q}}_j^{\perp}$ for $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m$; $j = 1, \dots, p$)
$RI_i^{\perp}$	Orthogonal representativeness index of LCI-result $\tilde{\mathbf{g}}_i$ for all orthogonalized impact categories ($i = 1, \dots, m$)
$RI_{j,\,i}^{\mathrm{decorr}}$	Decorrelated representativeness index of $\tilde{\mathbf{q}}_j$ for $\tilde{\mathbf{g}}_i$ ($i = 1, \dots, m$; $j = 1, \dots, p$)
SRR_j	Sum of squared correlation coefficients of $\tilde{\mathbf{q}}_j$ and all other $\tilde{\mathbf{q}}$-vectors ($j = 1, \dots, p$)
Θ_j	A set of impact category vectors that are correlated to $\mathbf{q}_j$ and belonging to $\mathbf{Q}$ ($j = 1, \dots, p$)
S_i	Sum of squared RIs over $t = 1, \dots, p$ ($i = 1, \dots, m$)
k	Iteration round ($k = 2, \dots, p$)
$R_{t,\,i,\,k}$	RI result of the $\tilde{\mathbf{q}}_t$ for $\tilde{\mathbf{g}}_i$ and treated during the iteration k ($t = 1, \dots, p$; $i = 1, \dots, m$; $k = 2, \dots, p$)
$d_{j,\,i}$	Distance between $RI_{j,\,i}$ and $RI_{j,\,i}^{\perp}$ ($i = 1, \dots, m$; $j = 1, \dots, p$)
$\langle \mathbf{x},\mathbf{y} \rangle$	Inner product of vectors $\mathbf{x}$ and $\mathbf{y}$
$\lVert \mathbf{x} \rVert$	Norm (Euclidean length) of vector $\mathbf{x}$

each component x of such an LCI result vector, so the elementary flows $g_{x,\,i}$ that form $\mathbf{g}_i$, has its own accounting unit (e.g. kilogram, Becquerel, joule…), and within this vector space, no consistent inner product (which induces a norm) can be defined (Heijungs and Suh, 2002). In this perspective, it is useful to recall that the vector spaces that are usually employed in the engineering disciplines refer to 3-dimensional Euclidean space, in which vectors have a magnitude and a direction, and concepts such as angle and distance make sense. In non-metric vector spaces, vectors are more abstractly considered to be n-tuples, for which such concepts are not defined (Gentle, 2007). In order to be able to measure distances or angles between vectors, we here extend the studied vector space with an inner product after a standardization step.

Among the diversity of possible standardizations (min-max, z-score…), the geometric mean of each elementary flow over all products is used in the present work for two reasons. First, the geometric mean is robust to extreme values. Secondly and more importantly, this choice allows our approach being free of the reference flow values of LCI results (i.e. the issue emphasized by Heijungs (2017) about Steinmann et al. (2017) approach; see the Section 2.1.2. and SI A.1 for details). Defining G_x as the geometric mean of the xth elementary flow, so

$$G_x = \exp\left(\frac{1}{m}\sum_{i=1}^{m} \ln\left|g_{x,i}\right|\right) \tag{1}$$

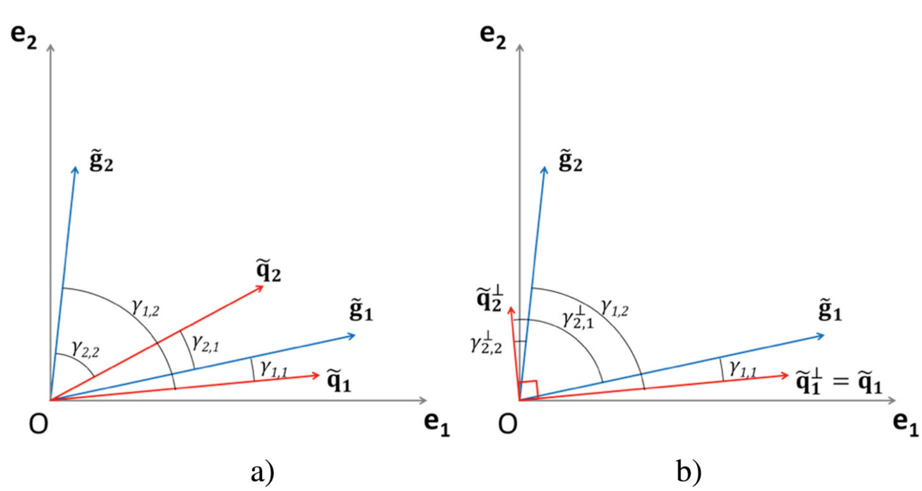

Fig. 1. a) Representation of two standardized LCI result vectors $\tilde{\mathbf{g}}_1$ and $\tilde{\mathbf{g}}_2$ (in blue), two standardized impact category vectors $\tilde{\mathbf{q}}_1$ and $\tilde{\mathbf{q}}_2$ (in red), and the four of the angles $\boldsymbol{\gamma}_{j,\,i}$ used to measure RIs. The vector space is spanned by two basis vectors ($\mathbf{e}_1$ and $\mathbf{e}_2$) representing standardized elementary flows, such as CO_2 and NO_x. b) Illustration of the correlation issue and $\tilde{\mathbf{q}}_2^{\perp}$, the orthogonal version of $\tilde{\mathbf{q}}_2$ (see below).

the x^{th} standardized elementary flows $\tilde{\mathbf{g}}_{x,i}$ of the ith LCI result is:

$$\tilde{g}_{x,i} = \frac{g_{x,i}}{G_x} \tag{2}$$

Note that we used the absolute value in Eq. (1) to allow for cases where the values are negative.

Within this standardized vector space and given two LCI result vectors $\tilde{\mathbf{g}}_1$ and $\tilde{\mathbf{g}}_2$, we can define the inner product of these vectors as:

$$\langle \tilde{\mathbf{g}}_1, \tilde{\mathbf{g}}_2 \rangle = \sum_{x=1}^{n} \tilde{g}_{x,1} \tilde{g}_{x,2} \tag{3}$$

Next, we define the norm or Euclidean length of a vector $\tilde{\mathbf{g}}_i$ as

$$\|\tilde{\mathbf{g}}_i\| = \sqrt{\langle \tilde{\mathbf{g}}_i, \tilde{\mathbf{g}}_i \rangle} \tag{4}$$

Finally, this allows us to define the angle α between two LCI vectors, say, $\tilde{\mathbf{g}}_1$ and $\tilde{\mathbf{g}}_2$, indicated by $\alpha_{1,\,2}$, as

$$\alpha_{1,2} = \arccos\left(\frac{\langle \tilde{\mathbf{g}}_1, \tilde{\mathbf{g}}_2 \rangle}{\|\tilde{\mathbf{g}}_1\| \|\tilde{\mathbf{g}}_2\|}\right) \tag{5}$$

Within the standardized vector space, the LCI result of each product has then its own vector direction and norm (see Fig. 1.a).

The norm of a standardized LCI result vector still depends on the magnitude of the reference flow of the product, while the direction of the vector doesn't. This justifies the proposed definition based on the angle between vectors (see Section 2.1.2).

Regarding impact categories, the consequences of unit amounts of the different elementary flows are summarised by their characterization factors (CFs), the numbers $q_{x,\,j}$. CFs are conversion factors used to assess the elementary flows in terms of impact category results. The collection of CFs of one impact category therefore defines a vector within the elementary flow vector space (according to the Fréchet-Riesz theorem, see Esnouf et al. (2018) Section 2.1.2). Fig. 1.a illustrates this for two impact categories, where the vector of CFs is denoted as $\tilde{\mathbf{q}}_1$ and $\tilde{\mathbf{q}}_2$, after standardization (see below).

Because we work with standardized elementary flows, the CFs should be standardized as well to maintain unit consistency:

$$\tilde{q}_{x,j} = q_{x,j} G_x \tag{6}$$

In this way, by standardizing the impact categories, we can depict the vectors $\tilde{\mathbf{q}}_j$ into the same standardized vector space. It reveals the main dimensions that contribute to each of the modelled environmental issues.

The LCIA step of the LCA framework translates the LCI result $\mathbf{g}_i$ into a quantified LCIA result $h_{j,\,i}$. The scalar $h_{j,\,i}$ is the amount of impacts on the jth impact category for the ith product using a linear transformation:

$$h_{j,i} = \sum_{x=1}^{n} q_{x,j} g_{x,i} \tag{7}$$

The LCIA result of a standardized LCI result vector $\tilde{\mathbf{g}}_i$ with a standardized impact category $\tilde{\mathbf{q}}_j$ equals to the previous LCIA result $h_{j,\,i}$ of the unstandardized vectors:

$$\tilde{h}_{j,i} = \left\langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i \right\rangle = \sum_{x=1}^{n} q_{x,j} G_x \frac{g_{x,i}}{G_x} = h_{j,i} \tag{8}$$

We extend the definition of the inner product of two standardized LCI vectors, say, $\langle \tilde{\mathbf{g}}_1, \tilde{\mathbf{g}}_2 \rangle$ to the inner product of two standardized impact categories, say, $\langle \tilde{\mathbf{q}}_1, \tilde{\mathbf{q}}_2 \rangle$, and to the inner product of a standardized LCI vector and a standardized impact category $\langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i \rangle$ (previously used in Eq. (8) for the definition of the LCIA result $\tilde{h}_{j,i}$). This also allows us to define the norm of an impact category, $\|\tilde{\mathbf{q}}_j\|$, the angle between two impact categories, β, and the angle ($\gamma_{j,\,i}$) between an LCI vector $\tilde{\mathbf{g}}_i$ and an impact category vector, $\tilde{\mathbf{q}}_j$. This finally allows us to define the representativeness index RI between an LCI vector and an impact category, as discussed in the next section.

2.1.2. RI between a LCI result and an impact category

Within a standardized vector space, the representativeness index (RI) proposed by Esnouf et al. (2018) is a measure between a standardized LCI result ($\tilde{\mathbf{g}}_i$) vector and an impact category vector ($\tilde{\mathbf{q}}_j$). In order to be free of the norm of the different vectors, it is based on the angle $\gamma_{j,\,i}$ between an LCI result vector and an impact category vector. The RI of an LCI result $\tilde{\mathbf{g}}_i$ for the impact category $\tilde{\mathbf{q}}_j$ is:

$$RI_{j,i} = RI\left(\tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i\right) = \left|\cos\left(\gamma_{j,i}\right)\right| = \left|\frac{\left\langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i \right\rangle}{\|\tilde{\mathbf{q}}_j\| \|\tilde{\mathbf{g}}_i\|}\right| = \left|\frac{\mathbf{h}_{j,i}}{\|\tilde{\mathbf{q}}_j\| \|\tilde{\mathbf{g}}_i\|}\right| \tag{9}$$

The higher the values of the RI, the better the impact category represents the main dimensions of the LCI result vector (i.e. the direction), relatively to the cumulated LCI database. Within the standardized vector space, the representativeness index can then be interpreted as a measure of similarity between the standardized LCI result vector and the standardized impact category vector.

2.1.3. RI between a LCI result and a LCIA method

In addition to the RI between an LCI result and an impact category, we define the RI between an LCI result and an entire LCIA method consisting of a collection of impact categories. An LCIA method can be regarded as a sub-space of the standardized vector generated by the impact categories. The LCIA method is written as a matrix $\mathbf{Q}$, consisting of the p different impact categories that belong to that method:

$$\mathbf{Q} = \left(\mathbf{q}_1 \ \cdots \ \mathbf{q}_p\right) \tag{10}$$

Because we decided to work in standardized space, we effectively work with

$$\tilde{\mathbf{Q}} = (\tilde{\mathbf{q}}_1 \quad \cdots \quad \tilde{\mathbf{q}}_p) \tag{11}$$

The RI of the entire LCIA method is then defined, for LCI result $\mathbf{g}_i$, as

$$RI_i = RI\left(\tilde{\mathbf{Q}}, \tilde{\mathbf{g}}_i\right) = \sqrt{\sum_{j=1}^{p} \left(RI\left(\tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i\right)\right)^2} \tag{12}$$

2.1.4. Correlation and decorrelation

The impact category vectors of the LCIA method are in general not orthogonal, that is, the angle β between some of the (standardized) impact category vectors is not 90 degrees. This also implies that for an LCIA method, subsets of non-orthogonal impact category vectors can be observed for which the impact category vectors are correlated with each other. The effect of this is an over- or under-representation of the LCI result vector by those impact category vectors. It relies on the fact that RIs of the non-orthogonal impact category vectors for the LCI result vector will assess and represent the LCI result vector through the same main elementary flows. Indeed, the main direction of a LCI result vector can be close to the main direction of two (or more) non-orthogonal impact category vectors, which lead to an over-representation, or at the opposite, both impact category vectors miss this main direction even if their characterization factors are not null on the main dimensions of the LCI result vector, which then lead to an under-representation. At the LCIA method level, this over or under-representation can be solved by an orthogonalization procedure of the impact category vectors $\tilde{\mathbf{q}}_j$ (Esnouf et al., 2018). This procedure is based on the well-known Gram-Schmidt process (Arfken and Weber, 2012). The Gram-Schmidt process returns a new set of standardized perpendicular vectors, which will be denoted here as $\tilde{\mathbf{q}}_j^{\perp}$ (see Fig. 1.b). Similar to Eq. (11), we can pack these vectors for the entire LCIA method in one matrix, $\tilde{\mathbf{Q}}^{\perp}$. Using the angle $\gamma_{j,i}^{\perp}$ between an LCI result vector $\tilde{\mathbf{g}}_i$ and an orthogonalized impact category vector $\tilde{\mathbf{q}}_j^{\perp}$, this in turn can serve to calculate a new RI of a LCIA method, similar to Eqs. (9) and (12):

$$RI_{j,i}^{\perp} = RI\left(\tilde{\mathbf{q}}_j^{\perp}, \tilde{\mathbf{g}}_i\right) = \left|\cos\left(\gamma_{j,i}^{\perp}\right)\right| \tag{13}$$

and

$$RI_i^{\perp} = RI\left(\tilde{\mathbf{Q}}^{\perp}, \tilde{\mathbf{g}}_i\right) = \sqrt{\sum_{j=1}^{p}\left(RI_{j,i}^{\perp}\right)^2} \tag{14}$$

The procedure that is proposed to take into account the over or under-representation for the RIs of impact category belonging to the same LCIA method is schematized in Fig. 2. The upper part describes the steps that are needed to obtain RI_i and $RI_i^{\perp}$ that are needed to take out the consequences of the correlations between impact category vectors. The lower part describes the iterative loop developed in Section 2.1.5. that is needed to solve the consequences triggered by the order dependency of the impact category that is inherent in the Gram-Schmidt process.

The Gram-Schmidt process allows obtaining a set of orthogonal impact category vectors from one LCIA method and thus allows determining its $RI_i^{\perp}$. But the order of processing the different $\tilde{\mathbf{q}}_j$ vectors in $\tilde{\mathbf{Q}}$ determines the RIs of the standardized and orthogonalized vectors. With the Gram-Schmidt iterative process, the first treated vector is not modified (and its RIs will not be different between $\tilde{\mathbf{q}}_1$ and $\tilde{\mathbf{q}}_1^{\perp}$) while the next vectors are orthogonalized paying regard to the previously handled vectors (and there will be differences between the RIs of $\tilde{\mathbf{q}}_j$ and $\tilde{\mathbf{q}}_j^{\perp}$ (for $j = 2, \ldots, p$)). Because of that, the orthogonalized impact category vectors that result from the Gram-Schmidt process cannot be directly used to look at the RIs of $\tilde{\mathbf{g}}_i$ for uncorrelated impacts due to this order dependency.

To solve the problem of order-dependency we define a unique order of treatment of the impact categories. Instead of applying Gram-Schmidt to the usual order $j = 1, \ldots, p$, we first sort the impact category vectors, and apply the Gram-Schmidt process to the vectors arranged in that new order. This order is determined by using the correlation matrix of the impact category vectors belonging to $\tilde{\mathbf{Q}}$ (see Fig. 2). This makes sense because the correlation coefficient of two vectors is equivalent to the cosine of the angle between these vectors (Gniazdowski, 2013), which in turn is equal to the RI as defined above. For each impact category, the sum of the squares of all its correlation coefficients (SSR) is calculated:

$$SSR_j = \sum_{l=1}^{p}\left(r\left(\tilde{\mathbf{q}}_j, \tilde{\mathbf{q}}_l\right)\right)^2 \tag{15}$$

This includes the trivial case $l = j$, for which $r = 1$, but because it doesn't affect the ranking we can leave it in. The order of impact categories is determined by ranking these sums SSR_j in descending order. The first impact category to be processed is then the one which has the highest SSR, and the maximal correlation with the other impact categories.

The over- or under-representation of an LCI result vector by a set of impact category vectors corresponds to the difference between the RIs measured by the non-orthogonal impact categories and the RIs

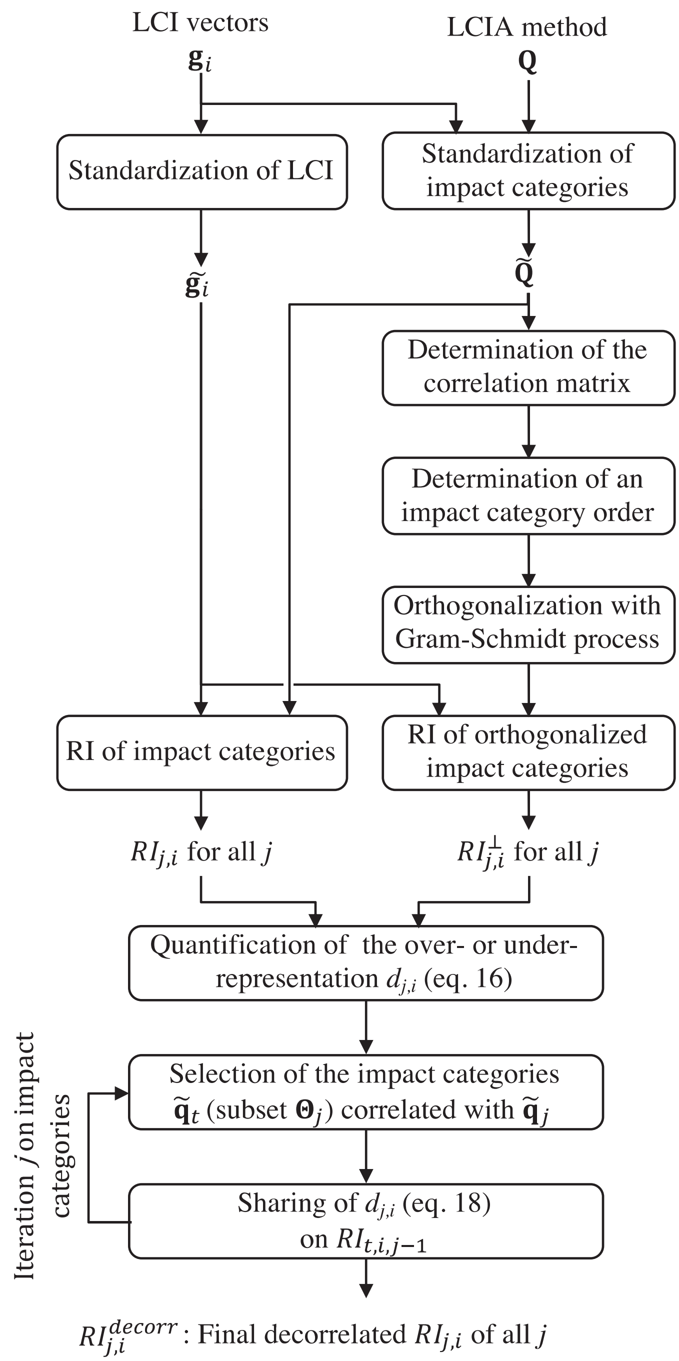

Fig. 2. Schematics of the proposed algorithm.

measured by the orthogonalized impact categories. Based on the determination of those differences, a decorrelation algorithm is proposed in the next section. This algorithm allows distributing the over- or under-representation between the non-orthogonal impact categories (iteration loop in Fig. 2).

2.1.5. Decorrelation algorithm of impact category RIs

From the $RI_{j,i}^{\perp}$ determined for a LCIA method after the Gram-Schmidt process, the over- or under-representation need to be quantified and distributed over the subset of non-orthogonal impact categories. For the LCI vector $\tilde{\mathbf{g}}_i$ and the impact category $\tilde{\mathbf{q}}_j$, the RI of the orthogonalized impacts ($RI_{j,i}^{\perp}$) is compared to the original one ($RI_{j,i}$). Their distance $d_{j,i}$ (as defined in Eq. (16)) is interpreted as the over- or under-representation of $\tilde{\mathbf{g}}_i$ expressed by the impact category j and that is redundant or missing regarding the categories that have been previously processed given the order of the impact categories used in the Gram-Schmidt process:

$$d_{j,i} = \sqrt{\left(RI_{j,i}\right)^2 - \left(RI_{j,i}^{\perp}\right)^2} \quad (16)$$

The over- or under-representation $d_{j,\ i}$ of the impact category $\tilde{\mathbf{q}}_j$ has to be distributed over the other non-orthogonal impact categories. For this purpose, each $d_{j,\ i}$ is treated iteratively with the same order that is used for impact categories in the Gram-Schmidt process. Let Θ_j be the subset of the category vectors $\tilde{\mathbf{q}}_t$ that are correlated to $\tilde{\mathbf{q}}_j$, $\Theta_j = \{\tilde{\mathbf{q}}_t | t \in \{1, \dots, p\}, r(\tilde{\mathbf{q}}_t, \tilde{\mathbf{q}}_j) \neq 0\}$. $RI_{t,\ i,\ j}$ is the RIs modified by the decorrelation process of the LCI result vector $\tilde{\mathbf{g}}_i$ for the impact category $\tilde{\mathbf{q}}_t$ during the jth iteration. For the first impact category treated $d_{1,\ i} = 0$ ($RI_{1,\ i}^{\perp}$ is equal to $RI_{1,\ i}$ because $\tilde{\mathbf{q}}_1$ is not modified by the Gram-Schmidt process, so $\tilde{\mathbf{q}}_1^{\perp} = \tilde{\mathbf{q}}_1$). Consequently, the results $RI_{t,\ i,\ 1}$ of $\tilde{\mathbf{g}}_i$ for these categories $\tilde{\mathbf{q}}_t$ are the original RIs that are obtained from Eq. (9):

$$RI_{t,i,1} = RI_{t,i} \quad (17)$$

Let $S_i = \sum_{t=1}^{p} \left(RI_{t,i,1}\right)^2$ the sum of the squares of $RI_{t,\ i,\ 1}$. For the following iterations ($j = 2, \dots, p$), all the $RI_{t,\ i,\ j}$ will share the over or under-representation measured by $d_{j,\ i}$:

$$RI_{t,i,j} = \sqrt{\left(RI_{t,i,j-1}\right)^2 - \left(d_{j,i}\right)^2 \times \frac{\left(RI_{t,i,1}\right)^2}{S_i}} \quad (18)$$

At the end of the iteration procedure, all the resulting decorrelated RIs, $RI_{j,\ i}^{decorr} = RI_{t,\ i,\ p}$, of $\tilde{\mathbf{g}}_i$ for the impact category vectors of an LCIA method obtained through this algorithm are free from the consequences of the order of the impact category used within the Gram-Schmidt process.

2.2. Material

The methodology is applied to the cumulated LCI result version of the ecoinvent 3.1 "allocation at the point of substitution" database (Wernet et al., 2016). This version of the cumulated LCI database was released in 2014. It comprises 11,206 LCI result vectors that are described through 1727 elementary flows (the intervention matrix). The elementary flows vector space therefore has 1727 dimensions. Compared to Esnouf et al. (2018), the same matrix was used although certain elementary flows and LCI results were removed from the cumulated LCI database. Indeed, considering that the analysis is applied to LCI results, the 70 LCI results that have only less than 30 referenced elementary flows are set aside. 142 elementary flows were also not taken into account due to the low number of LCI results that take value on them.

The ILCD V1.05 (EC-JRC, 2010a) is the studied LCIA method. It was extracted from the SimaPro 8.1.1.16 software to analyse the most recent and operational version. The CF nomenclature was transferred from the SimaPro nomenclature to the ecoinvent elementary flows nomenclature with the assistance of the ecoinvent centre.

Implementation was conducted with Python 2.7 on a Jupyter Notebook (Perez and Granger, 2007) (formerly IPython Notebook) and using numerical computation libraries SciPy (V 0.16.0), Pandas (V 0.17.1) and Matplotlib (V 1.5.0). Python is an open-source programming language which is increasingly used in data sciences and in LCA framework as in Brightway2 (Mutel, 2017).

An operational tool written with Python 3.6 was also developed. It is available from an online deposit hosted on github.com with the DOI: https://doi.org/10.5281/zenodo.1068914. The package allows to apply the methodology on LCI result excel files (system process) exported from SimaPro and modelled within the ecoinvent 3.1 "allocation at the point of substitution" database (further development needs to be done to apply the methodology to other cumulated LCI databases and to cumulated LCI result files exported from other software). Three outputs can be obtained per LCI result: RIs of LCIA methods, RIs of their impact category vectors and RIs of decorrelated categories. Almost all the multi-criteria LCIA methods can be analysed. Standardization is applied with geometric means of elementary flows after a nomenclature translation from ecoinvent to SimaPro.

Based on the studied cumulated LCI ecoinvent database, the LCI results of the Chinese and the German electricity production mixes serve as an illustrative example of the presented work. The two LCI results refer to the market production of 1 kWh of high voltage electricity. The market version of these LCI results models the elementary flows of electricity production mixes, transmission networks and electricity losses during transmission.

3. Results and discussion

3.1. Illustrative example

3.1.1. LCIA results analysis with respect to RIs

A comparison of LCIA results from the Chinese and the German electricity mixes points to a number of noteworthy elements evidenced by the impact categories RI results (see Fig. 3). The upper bar-chart typically illustrates the results of a comparative LCA study, the lower chart represents the outputs of the python package (see data in SI B). For the German mix, ten impact category results are higher than for the Chinese mix, out of the sixteen impact categories of the ILCD method. Germany is two-fold higher for 9 categories: Ozone depletion, Toxicities (cancer and non-cancer effects), Ionizing radiations (human health and ecosystems), Freshwater eutrophication, Ecotoxicity and both Resource depletions. The German mix also uses a higher proportion of land area, but the gap is smaller (China is only 21% lower than Germany on this impact category). Contrasting LCIA results are observed for particulate matter, photochemical ozone formation, acidification and terrestrial eutrophication where China is five times higher than Germany. The same observation can be made for climate change and marine eutrophication but with a lower difference (compared to China, German impacts are lower by 41% and 63% respectively).

The global RIs of the ILCD method are 0.113 for the Chinese and 0.0285 for the German mix. The Chinese mix has a better overall representation with this LCIA method because its RI of method is higher. Using impact category RIs from Fig. 3, this high overall RI of the method comes from high impact category RI results on particulate matter, acidification, photochemical ozone formation, climate change and terrestrial eutrophication (in decreasing order of contribution). During interpretation, the focus must, in priority, be put on this reduced set of impact category vectors.

The main representative impact categories for the German mix are ionizing radiation (HH), freshwater eutrophication, climate change, water resource depletion and human toxicity (non-cancer effect). The RIs of these LCIA results are two to three times higher for these impact categories (see Fig. 3) and they should be looked at first and foremost for the result interpretation.

The environmental issues highlighted for this comparative LCA study are not the same for both LCI results. Given the contextualization of LCI results and impact categories from the cumulated LCI database, the use of $RI_{j,\ i}$ and $RI_{j,\ i}^{\perp}$ guides the LCA practitioner in the interpretation of the main representative impact categories for each LCI result.

3.1.2. Example of decorrelation on two LCI results

Results from the decorrelation of impact category RI results obtained for the two previously studied LCI results are presented in Fig. 3. Using the $RI_{j,\ i}$, Eq. (12) results in 0.137 and 0.0293, respectively for the Chinese and the German mixes, while the overall RIs of the ILCD method are 0.113 and 0.0285 (see above). These differences a dependence

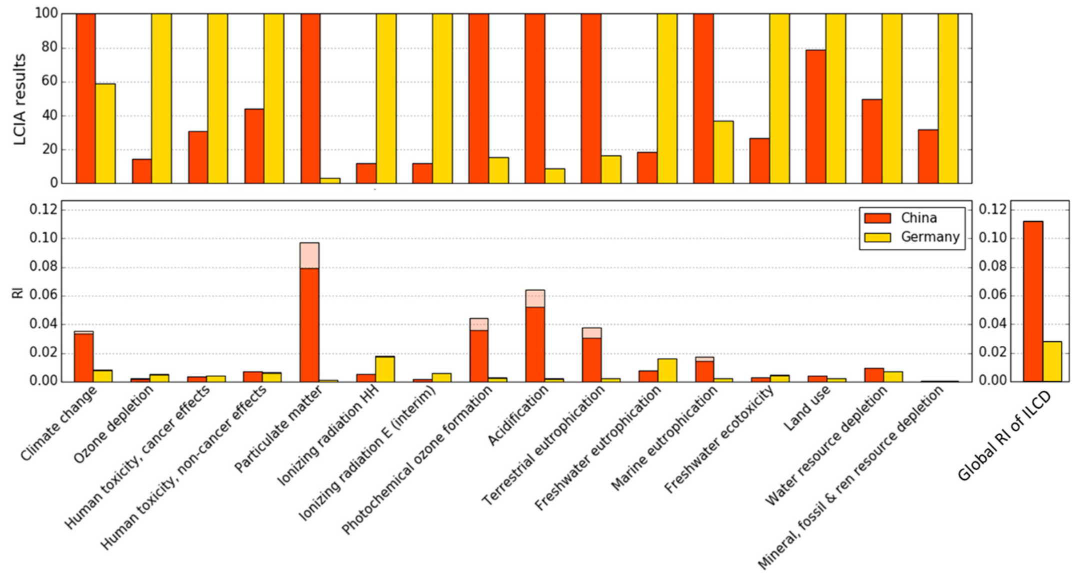

Fig. 3. LCIA results (expressed relative to the highest value) and impact category RIs for the LCI results of the Chinese and German electricity mixes from the ILCD method. Bright colours correspond to decorrelated RIs $\boldsymbol{RI}_{j,i}^{\mathbf{decorr}}$ while pastels colours indicate the part removed from the original RIs by the decorrelation procedure, $\boldsymbol{d}_{j,i}$.

between the impact category vectors, which are removed by the presented algorithm.

Six impact category RIs are particularly affected by decorrelation (see Fig. 3). The algorithm lowers the representativeness index of the Chinese mix for the particulate matter, acidification, photochemical ozone formation, and terrestrial eutrophication categories. The climate change and marine eutrophication categories are affected to a lesser extent. The decorrelation of the German mix RIs does not affect its representativeness index on any particular impact category. Orthogonalized results do not modify the previous interpretations.

3.2. Global trends of impact category RIs over the cumulated LCI database

The ordered distribution of the impact category RIs of the entire cumulated LCI database indicates that their values rapidly decrease below 0.1, reaching 10^{-2} to 10^{-5} (see Fig. 4). These low values result from the high-dimensional vector space in which the study takes place. The ranges of impact category RI values are globally similar when the different impact categories are compared. In an analogous manner, these impact categories represent the different LCI results of the cumulated database, in terms of quantity of information. They all seem relevant for a large number of LCI results. However, all impact categories are probably not compulsory for the analysis of a single LCI result, as observed in the previous illustrative example.

3.3. Decorrelation of impact category RIs within a LCIA method

3.3.1. Correlation matrix of impact categories

Table 2 presents the correlation matrix of the impact categories (after standardization). Based on their correlation, five different subsets of intercorrelated categories (i.e. Θ_j) are labelled from A to E and described in Table 3. Some impact categories feature in two subsets.

The Photochemical ozone formation (within subset C) has a particular position because it correlates with the two subsets A and B which do not have any elementary flows in common. This category is the one with the highest *SSR* (Eq. (15)) and is therefore the first one to be processed by the algorithm. Consequently, the orthogonalization of one subset A or B does not affect the orthogonalized RI of the other subsets through Photochemical ozone formation relationships. However, the Photochemical ozone formation is affected by both subset A and B.

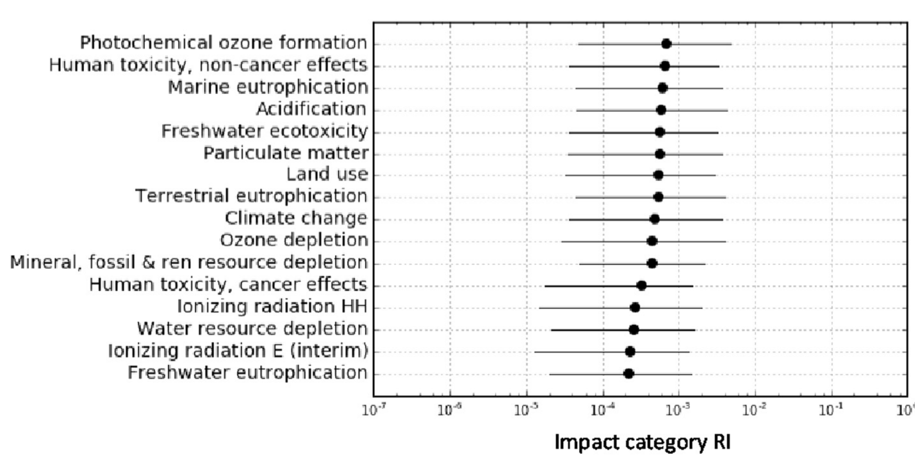

Fig. 4. Range of RI values of the ILCD impact categories regarding the 11,206 LCI results of ecoinvent. Shown are: the median (dot), the first quartile (left end of line) and third quartile (right end of line). Impact categories are sorted according to their median.

Table 2
Correlation matrix of impact categories of the ILCD method, on the basis of 11,206 products from ecoinvent.

	FWET	HTC	HTNC	ODP	CCP	MEP	TEP	AP	PMP	POFP	IRE	IRHH	MFRDP	WRDP	LU	FWEP
FWET	1	5.3e−1	9.5e−2	2.9e−11	1.4e−13	0	0	0	0	4.0e−9	0	0	0	0	0	0
HTC	5.3e−1	1	1.0e−2	2.0e−7	6.0e−11	0	0	0	0	1.4e−8	0	0	0	0	0	0
HTNC	9.5e−2	1.0e−2	1	1.4e−7	2.9e−11	0	0	0	0	2.6e−7	0	0	0	0	0	0
ODP	2.9E−11	2.0e−7	1.4e−7	1	9.1e−5	0	0	0	0	6.2e−11	0	0	0	0	0	0
CCP	1.4e−13	6.0e−11	2.9e−11	9.1e−5	1	0	0	0	0	1.2e−3	0	0	0	0	0	0
MEP	0	0	0	0	0	1	4.4e−1	1.5e−1	1.2e−2	4.3e−1	0	0	0	0	0	0
TEP	0	0	0	0	0	4.4e−1	1	3.4e−1	2.7e−2	9.7e−1	0	0	0	0	0	0
AP	0	0	0	0	0	1.5e−1	3.5e−1	1	3.3e−1	4.5e−1	0	0	0	0	0	0
PMP	0	0	0	0	0	1.2e−2	2.7e−2	3.3e−1	1	6.7e−2	0	0	0	0	0	0
POFP	4.0e−9	1.4e−8	2.6e−7	6.2e−11	1.2e−3	4.3e−1	9.7e−1	4.5e−1	6.7e−2	1	0	0	0	0	0	0
IRE	0	0	0	0	0	0	0	0	0	0	1	5.7e−1	0	0	0	0
IRHH	0	0	0	0	0	0	0	0	0	0	5.7e−1	1	0	0	0	0
MFRDP	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0
WRDP	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
LU	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
FWEP	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1

The two ionizing radiation impact categories (subset D) are only correlated with each other. Impact categories that do not correlate with any other are gathered in subset E.

The correlation coefficients point out that subsets B and D present very high correlations (between 1.17×10^{-2} and 4.44×10^{-1}) in comparison to subset A (from 1.40×10^{-13} to 5.32×10^{-1}). The Photochemical ozone formation potential also presents higher correlation coefficients with subset B (up to 9.66×10^{-1}) than with subset A (up to 1.24×10^{-3}).

3.3.2. Consequences of decorrelation over the cumulated LCI database

Orthogonalized impact category RI values are obtained by applying the algorithm to all 11,206 ecoinvent LCI results. To determine the global trends of the redistribution of the representativeness of impact categories for all LCI results, the distribution of the ratio $\frac{RI^{decorr} - RI}{RI}$ are analysed for each impact category; see Fig. 5. Distributions of the ratio are based on the original RI values and the orthogonalized RI values of the impact categories (see Eqs. (16) and (18)). For one LCI result, all the RIs of the impacts categories with a similar belonging to the subsets obtain the same ratio (while each LCI result is associated to a unique ratio). That means with the ILCD method that five group are done: Impact categories only in subset A, only in subset B, in A, B and C (i.e. the Photochemical ozone formation category), in D and in E.

Table 3
Definition of subsets of impact categories and their abbreviations.

Impact category	Abbreviation	Member of subset A	B	C	D	E
Freshwater ecotoxicity	FWET	X		X		
Human toxicity, cancer effects	HTC	X		X		
Human toxicity, non-cancer effects	HTNC	X		X		
Ozone depletion	ODP	X		X		
Climate change	CCP	X		X		
Marine eutrophication	MEP		X	X		
Terrestrial eutrophication	TEP		X	X		
Acidification	AP		X	X		
Particulate matter	PMP		X	X		
Photochemical ozone formation	POFP	X	X	X		
IRE Ionizing radiation E (interim)	IRE				X	
Ionizing radiation HH	IRHH				X	
Mineral, fossil & renewable resource depletion	MFRDP					X
Water resource depletion	WRDP					X
Land use	LU					X
Freshwater eutrophication	FWEP					X

Results imply that the major part of the redistribution slightly decreases the RI values from $RI_{j,i}$ to $RI_{j,i}^{decorr}$ (between 0 and 20%). Obviously, impact categories that do not correlate with any other impact category do not show any change (subset E).

For subsets A, B and C, a decrease is the main tendency but high increases are observed for some inventories, with 95% percentiles up to 80% (reaching 300% for extreme values). High values are correlated between the impact categories of these 3 subsets (see SI A.2). However, for the major part of the impact category RIs (negative modifications down to −20%), the correlation appears to be less obvious. Nevertheless, the modifications remain low for each subset. The wide RI redistribution of the photochemical ozone formation (first impact category treated by the algorithm) is triggered by the orthogonalization from the other two subsets that form another "profile" on Fig. 5.

As for subset D, the distribution of the modifications in impact category RI is very restricted. This could be explained by the fact that only two impact categories belong to this subset. No correlation of the redistribution with the other subsets is observed (see SI A.2).

The increase of RI values for $RI_{j,i}^{decorr}$ is triggered by the high $RI_{j,i}^{\perp}$ which is observed for several subsets. A LCI result with a high value on an elementary flow, which is not associated to a high CF of any impact categories, can be highlighted by the orthogonalization step and thus lead to an increase in the RI value. The orthogonalization of the impact category redirects the vector towards a secondary elementary flow (see Fig. 1.b). When LCI results have a high value on this second elementary flow, their $RI_{j,i}^{\perp}$ tends to increase compared to $RI_{j,i}$. Most of the LCI results characterized by higher $RI_{j,i}^{\perp}$ originate from agricultural production. This is mainly related to ammonia and nitrate elementary flows. The redistribution of extra information from the secondary elementary flow should provide the impact categories of the subset with an increase that finally allows their $RI_{j,i}^{decorr}$ to comply with the RI of the LCIA method.

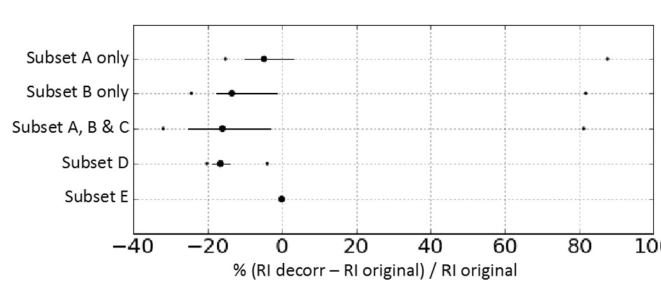

Fig. 5. Analyses of the different redistribution of RI values. Ordinate refers to the belonging of the impact categories. Shown are: the median (large dot), the first quartile (left end of line), the third quartile (right end of line), and the 5% and 95% percentiles (small dots).

4. Conclusions

This work completes the RI methodology previously developed (Esnouf et al., 2018) by focusing on the appropriateness of impact categories. We propose a freely downloadable operational tool for RI calculation and have applied this methodology to an illustrative example. The impact category RIs have proven that interpretations of LCIA results can be deepened. They can assist practitioners by orientating their analysis towards relevant impact categories. Analyses were also carried out over all LCI results of the cumulated LCI database to extract global RI trends. The same approach could also be used for other ecoinvent versions, cumulated LCI databases or specific fields of activity. Moreover, the cumulated LCI database trends were used here to standardize the impact categories. Other types of standardization, for example, based on the global elementary flows of a geographical area or economic sector, could relate the RI methodology. Finally, a focus on the standardized elementary flows that provide the value of the impact category RIs for each LCI result could be interesting to trace the main directions that are linked to each impact category.

An algorithm proposing a solution for correlation issues was developed and implemented within the operational tool. Redundant information was spread out according to the original impact category RI. Further work could focus on other types of algorithms where the whole impact category subset would not be affected by the modification of RIs. Only the impact categories with elementary flows affected by orthogonalization would be affected. Based on the RI methodology and taking into account the consistency of impact categories, relevant impact categories could also derive from different LCIA methods, thus enabling the development of composite LCIA methods.

Conflict of interest

The authors declare no conflict of interest.

Funding

This work was supported by the Clean, Secure and Efficient Energy societal challenge of the French National Research Agency, under contract GreenAlgOhol ANR-14-CE05-0043.

Acknowledgment

The authors acknowledge the ecoinvent centre for help provided on database description and data-pretreatment.

Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2018.12.194.

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