Representativeness of environmental issues regarding Life Cycle Inventory of products - Toward the development of an innovative metric

Antoine Esnouf

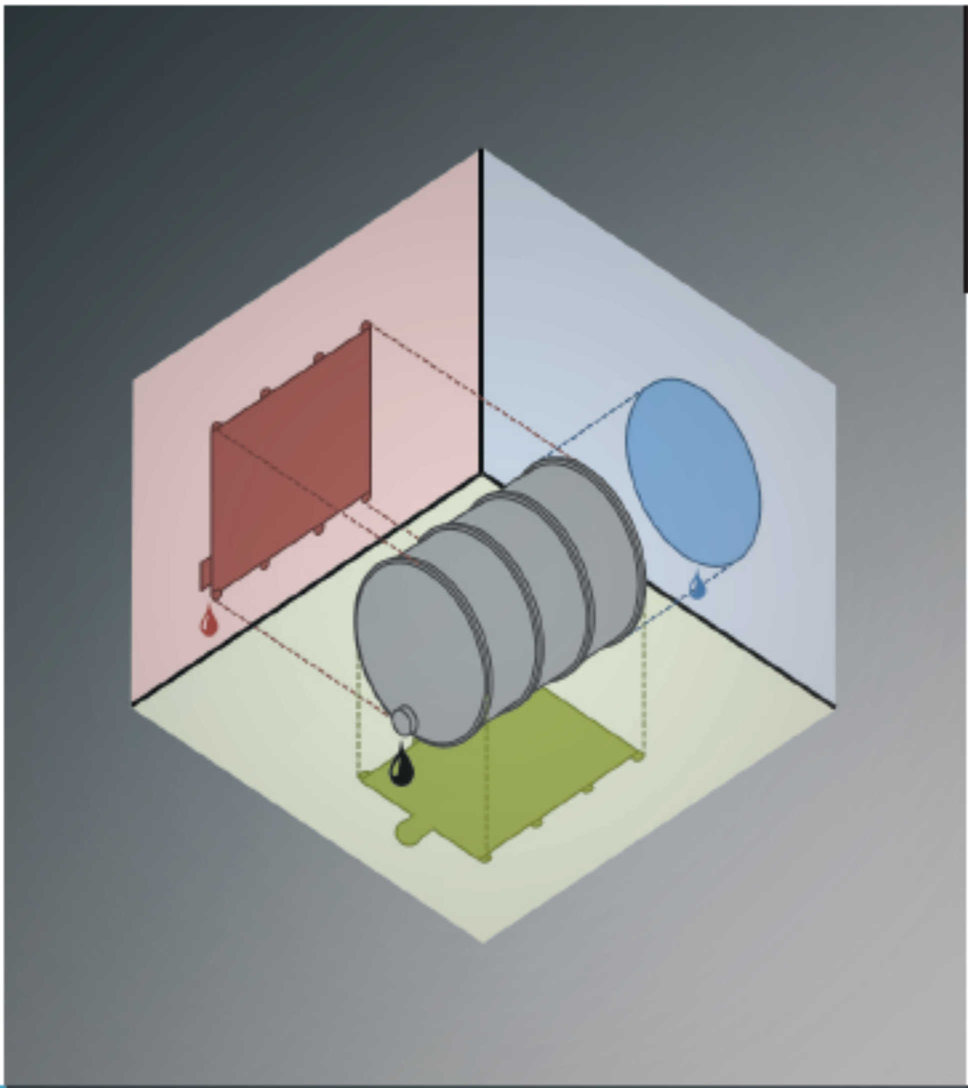
To cite this version:

Antoine Esnouf. Representativeness of environmental issues regarding Life Cycle Inventory of products - Toward the development of an innovative metric. Life Sciences [q-bio]. Institut National d'Etudes Supérieures Agronomiques de Montpellier; Université de Montpellier, 2018. English. NNT : . tel-02789802

HAL Id: tel-02789802
https://hal.inrae.fr/tel-02789802v1

Lbe

Antoine ESNOUF



PhD thesis 2018

REPRÉSENTATIVITÉ DES PROBLÉMATIQUES ENVIRONNEMENTALES AU REGARD DES INVENTAIRES DU CYCLE DE VIE DE PRODUITS

DÉVELOPPEMENT D'UNE MÉTRIQUE INNOVANTE

REPRESENTATIVENESS OF ENVIRONMENTAL ISSUES
REGARDING LIFE CYCLE INVENTORY OF PRODUCTS -
TOWARD THE DEVELOPMENT OF AN INNOVATIVE METRIC

INRA
SCIENCE & IMPACT

Membre fondateur de
agreenium

THÈSE POUR OBTENIR LE GRADE DE DOCTEUR DE MONTPELLIER SUPAGRO

En Génie des procédés

École doctorale GAIA – Biodiversité, Agriculture, Alimentation, Environnement, Terre, Eau
Portée par l'Université de Montpellier

Unité de recherche INRA – Laboratoire de Biotechnologie de l'Environnement

Representativeness of environmental issues regarding Life Cycle Inventory of products

-

Toward the development of an innovative metric

Présentée par Antoine ESNOUF
Le 31 mai 2018

Sous la direction de Arnaud HELIAS

Devant le jury composé de

Ligia Barna, Professeure, INSA Toulouse	Rapportrice
Isabelle Blanc, Directrice de Recherche, MINES ParisTech	Rapportrice
Reinout Heijungs, Associate professor, Vrije Universiteit Amsterdam	Examinateur
Arnaud Hélias, Maître de conférences, Montpellier SupArgo	Directeur de thèse
Eric Latrille, Ingénieur de recherche, INRA	Membre invité
Philippe Loubet, Maître de conférences, ENSCBP-Bordeaux INP	Examinateur
Ronan Pierre, Docteur, CEVA	Membre invité
Jean-Philippe Steyer, Directeur de Recherche, INRA	Examinateur et président du jury

UNIVERSITÉ DE MONTPELLIER

Montpellier SupAgro

Abstract / Résumé

The Life Cycle Assessment framework (LCA) is a multi-criteria approach aiming to assess all the potential environmental impacts of any human activities. Within a standardized framework, a human activity is described throughout its values chain: from raw material extraction, through materials processing, distribution, use stages, to waste management. Then, all emission flows to the environment as well as all resource consumption flows, all defined as elementary flows, are quantified in a Life Cycle Inventory result (LCI). Translation of LCI results into a reduced number of scores that each has an environmental meaning is carried out at the Life Cycle Impact Assessment (LCIA) phase using LCIA methods. However, the holistic nature of LCA, which has induced the development of many different LCIA methods with quite a few environmental impact categories each, can make the LCIA method and impact categories selection challenging for LCA practitioners. By benefiting from a huge compilation of LCI results within cumulated LCI database, the present work develops the Representativeness Index (RI) that assesses, from a geometrical point of view, the appropriateness of LCIA methods and their impact categories for any LCI result. This innovating approach relies on the contextualization of LCI results and impact categories regarding a database and on an angular measurement within a vector space. The relevance of the RI results is tested by analysing RI trends from an entire database and by applying it to a biofuel study case.

Keywords: Life Cycle Assessment, Life Cycle Inventory, Life Cycle Impact Assessment method, Representativeness, Angular distance, Dimension reduction, Biofuel

Le cadre d'Analyse du Cycle de Vie (ACV) est une approche multicritères visant à évaluer tous les impacts environnementaux potentiels de toute activité humaine. Dans un cadre normalisé, une activité humaine est alors décrite sur toute sa chaîne de valeurs (de l'extraction des matières premières, en passant par le traitement des matières premières, la distribution, les étapes d'utilisation et la gestion des déchets) et toutes les émissions vers l'environnement ainsi que toutes les consommations de ressources, aussi nommées flux élémentaires, sont quantifiées et regroupées dans un Inventaire du Cycle de Vie (ICV). La traduction des flux élémentaires en un nombre réduit de scores ayant chacun une signification environnementale est effectuée lors de la phase d'Evaluation de l'Impact sur le Cycle de Vie (EICV) à l'aide des méthodes d’EICV. Cependant, la nature holistique de l'ACV, qui a entrainé le développement de nombreuses méthodes d’ECVI avec chacune un certain nombre de catégories d'impact environnemental, peut rendre non évidente la sélection d’une méthode d’EICV et des catégories d'impact pour le praticien ACV. En bénéficiant de regroupement d'ICVs au sein de base de données, ce travail de thèse a permis de développer un Indice de Représentativité (IR) qui évalue, d'un point de vue géométrique, l'adéquation des méthodes d’ECVI et de leurs catégories d'impact pour un ICV donné. Cette approche innovante repose sur la contextualisation des ICVs et des catégories d'impact par rapport à une base de données d’ICVs et sur une mesure angulaire au sein d’un espace vectoriel. La pertinence des résultats de l'IR est testée en analysant leurs tendances au sein d'une base de données et en l'appliquant à un cas d'étude sur la production d’un agro-carburant à partir de macro-algue.

Mots-clés : Analyse du cycle de vie, Inventaire du Cycle de Vie, Méthode d’Évaluation de l’Impact du Cycle de Vie, Représentativité, Distance angulaire, Réduction de dimension, Agro-carburant

Remerciements

Il va être très difficile de remercier tout le monde car c'est avec l'aide de nombreuses personnes que j'ai pu mener cette thèse à son terme.

Tout d'abord, ce travail de thèse a été réalisé dans le cadre d'un financement ANR qui a regroupé cinq instituts recherche : le CEVA, le CERMAV, l'IFP Energies Nouvelles, l'ISCR et l'INRA à travers le LBE, mon laboratoire d'accueil. Je tiens à remercier toutes les personnes qui ont rendu possible ce projet, qui l'ont fait vivre et avec qui j'ai interagi durant ces trois années, notamment Ronan Pierre du CEVA qui en fut le coordinateur.

Je remercie les rapportrices de ce travail, Ligia Barna et Isabelle Blanc, ainsi que ses examinateurs, Reinout Heijungs, Philippe Loubet et Jean-Philippe Steyer pour les discussions, les commentaires et les améliorations qui en ont découlés.

Un grand merci à tous les membres de l'équipe ELSA, et particulièrement à mes co-bureaux Pyrène, Charlotte et Ariane. Je tiens aussi à remercier les membres de l'équipe du Génie Rural à Montpellier, ainsi que du LBE à Narbonne pour leur accueil malgré la distance.

Je tiens ensuite à remercier mes encadrants, Arnaud Hélias, Jean-Philippe Steyer et Eric Latrille pour leur rigueur, leur soutien, leur enthousiasme dans le déroulement de ce travail et surtout leur bonne humeur ! Je remercie aussi les membres de mon comité de thèse : Eléonore Loiseau, Jean-Denis Mathias, Jean-Michel Roger et Eric Trably.

Je remercie chaleureusement toute ma famille et mes amis qui m'ont supporté, encouragé et changé les idées durant toute cette aventure.

Merci à tous !

Preface

This thesis was supported by the Clean, Secure and Efficient Energy societal challenge of the French National Research Agency (ANR), under contract Green AlgOhol ANR-14-CE05-0043.

Green AlgOhol project began in January 2015 and ends in June 2018. It aims at evaluating the suitability and sustainability of a cellulosic macro-algae production as a raw material for bio-refinery. Five research partners are collaborating in this project:

- CEVA, Centre d'Etude et de Valorisation des Algues,
  coordinator of the project, in charge of biomass production and pre-treatment aspects;
- CERMAV, CEntre de Recherches sur les MAcromolécules Végétales,
  working on algae structure and composition;
- IFP-EN, Institut Français du Pétrole et des Énergies nouvelles,
  focused on pre-treatment step and hydrolysis alternatives;
- ISCR, Institut des Sciences Chimiques de Rennes,
  specialised on alcoholic fermentation;
- INRA – LBE, Institut National de la Recherche Agronomique – Laboratoire de Biotechnologie de l'Environnement,
  providing environmental assessment results, to ensure an efficient system design.

With this PhD work, INRA – LBE was in charge of the Life Cycle Assessment of the "seaweed to products" values chain developed in the project. Besides to the environmental assessment task, which is not explained here in detail, this thesis proposes a new approach for the selection of environmental indicators for LCA study. The manuscript is focused on this aspect, and as an illustration, the developed methodology was applied on the Green AlgOhol system.

During the PhD, the following papers were published or submitted in peer-reviewed journals:

- **Esnouf A**, Latrille E, Steyer JP, Helias A (2018). Representativeness of environmental impact assessment methods regarding Life Cycle Inventories. Science of the Total Environment. 621:1264-1271. IF (4.9) *(https://doi.org/10.1016/j.scitotenv.2017.10.102)*;
- **Esnouf A**, Heijungs R, Coste G, Latrille E, Steyer JP, Helias A. (2019) A tool to guide impact category selection for LCA studies by using the Representativeness Index. Science of the Total Environment. 658:768-776 IF (4.9) *(https://doi.org/10.1016/j.scitotenv.2018.12.194)*.

Articles in preparation:

- **Esnouf A**, Latrille E, Steyer JP, Helias A. Representativeness of impact categories in LCA according to fields of activity;
- **Esnouf A**, Pierre R, Aymard C, Latrille E, Steyer JP, Helias A. Life Cycle Assessment of a biofuel production from cellulosic macro-algae: key aspects for the environmental concerns.

In addition to this work, the following article was published during this PhD:

- Larrey-Lassalle P, **Esnouf A**, Roux P, Lopez-Ferber M, Rosenbaum R, Loiseau E (2018). A methodology to assess habitat fragmentation effects through regional indexes: illustration with forest biodiversity hotspots. Ecological Indicators. 89:543-551. IF (3.9).

This work also included oral communications and posters in international conferences:

Oral presentations

- **Esnouf A**, Latrille E, Steyer J.P, Helias A (May 2018). Which impact categories are relevant for LCA results interpretation? SETAC Europe 28th Annual Meeting, Roma;
- **Esnouf A**, Latrille E, Steyer J.P, Helias A (May 2017). Representativeness of LCIA methods regarding LCI. SETAC Europe 27th Annual Meeting, Brussels;
- Gabutti M, **Esnouf A**, Araniti N, L. Del Rio, Locatelli H, Pinheiro Silva S, Amrane A, Djelal H, Helias A (September 2016). Life cycle assessment of bioethanol from date waste in Tunisia. SETAC Europe 22nd Case Study Symposium, Montpellier.

Posters

- **Esnouf A**, Latrille E, Steyer J.P, Helias A (May 2016) Representativeness of environmental impacts in relation to Life Cycle Inventories. SETAC Europe, 26th Annual Meeting, Nantes;
- **Esnouf A**, Aissani L, Laurent F, Déchaux C (August 2015). Multifunctionality issue regarding LCA of bioenergy plants. 7th International Conference on Life Cycle Management, Bordeaux.

Lay abstract / Résumé pour le grand public

Human activities affect the environment through natural resources consumptions and polluting substances emissions. By quantifying these consumptions and emissions, also called elementary flows, Life Cycle Assessment is a standardized tool that evaluates the potential environmental impacts of a product throughout its life cycle. The translation of a product description into environmental impacts is then compulsory in order to be able to study and compare products on a limited number of indicators and not on all the identified flows. To this end, potentially disturbed environmental mechanisms have been modelled and improved over the past few decades. However, the choice of environmental indicators may not be obvious among all the proposed one, whereas this step is crucial for an environmental analysis. This thesis proposes the development of an innovative metric to support this choice and to question the relevance of the selected indicators.

Les activités humaines interviennent sur l'environnement à travers la consommation de ressources naturelles et l'émission de substances polluantes. Grâce à la quantification de ces consommations et émissions, aussi appelées flux élémentaires, l'Analyse du Cycle de Vie est un outil normalisé qui évalue les impacts environnementaux potentiels d'un produit sur tout le long de son cycle de vie. La traduction d'un produit en termes d'impacts sur l'environnement permet d'étudier et de comparer des produits sur un nombre restreint d'indicateurs et non sur l'ensemble des flux recensés. Pour cela, les mécanismes environnementaux potentiellement perturbés ont été modélisés et améliorés depuis quelques décennies. Cependant, le choix des indicateurs environnementaux peut ne pas être évident parmi tous ceux proposés alors que cette étape est cruciale pour une analyse environnementale. Cette thèse propose le développement d'une métrique innovante qui permet d'accompagner ce choix et d'interroger la pertinence des indicateurs sélectionnés.

Table of contents

Table of contents

Tables

Tables – Main Chapters

Tables – Supplementary Information

Figures

Figures – Main Chapters

Figures - Supplementary Information

Glossary

Frequent acronyms and abbreviations:

AF	Agriculture and Forestry
CF	Characterization Factor
EPG	Electricity Power Generation
HH	Human Health
ILCD	International Reference Life Cycle Data System
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
MATE	Machinery and transport equipment
PCA	Principal Component Analysis
RI	Representativeness Index
SACS	Steam and Air Conditioning Supply

Main variables, parameters and notations

Vectors and matrices are distinguished from scalar by being written in bold, matrices are moreover capitalized.

m	Number of products in LCI database
n	Number of elementary flows
p	Number of impact categories in a LCIA method
$\mathbf{G}$	$\mathbb{R}^n$ vector space where each dimension refers to an elementary flow
i	the i-th product of the cumulated LCI database
$\mathbf{g}_i$	LCI result vector of the i^{th} product $(i = 1, \dots, m)$
$g_{x,i}$	The amount of the x^{th} elementary flow for the i^{th} product $(i = 1, \dots, m; x = 1, \dots, n)$
j	the j-th characterization model of a LCIA method
$\mathbf{q}_j$	The vector of characterization factors of the j^{th} impact category within G^*: an impact category vector $(j = 1, \dots, p)$. It is also the impact category vector transferred from G^* to G

$q_{x,j}$	The characterization factor of the j^{th} impact category for the x^{th} elementary flow ($j = 1, \dots, p; x = 1, \dots, n$)
$\mathbf{G^*}$	Dual space of the **G** vector space, i.e. the $\mathbb{R}^n$ vector space of all the linear forms $q_j : G \to \mathbb{R}$
$\mathbf{Q}$	LCIA method matrix composed of a set characterization vectors of p impact categories
$h_{j,i}$	LCIA result of the i^{th} product on the j^{th} impact category ($i = 1, \dots, m; j = 1, \dots, p$)
G_x	Geometric mean of $g_{x,i}$ for the x^{th} 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 ($i = 1, \dots, m$)
$RI_{j,i}^{\perp}$	Ortohogonal 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 ($i = 1, \dots, m$)
$RI_{j,i}^{\text{decorr}}$	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 **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 $RI_{j,i}^{\perp}$ ($i = 1, \dots, m; j = 1, \dots, p$)
$I_{j,i}$	Projection of the $\tilde{\mathbf{g}}_i$ LCI vector on the $\tilde{\mathbf{q}}_j$ impact category vector
$\alpha_{j,i}$	Angle formed by the directions of $\tilde{\mathbf{g}}_i$ LCI and the impact category vector $\tilde{\mathbf{q}}_j$
$\lvert\cos(\alpha_{j,i})\rvert$	Absolute value of the angular cosine of $\alpha_{j,i}$
$\langle \mathbf{x}, \mathbf{y} \rangle$	Inner product of vectors **x** and **y**
$\lVert\mathbf{x}\rVert$	Norm (Euclidean length) of vector **x**

Additional definitions:

Elementary flow intensity: after the standardization procedure (Chapter 2), the intensity refers to the contribution of the elementary flow on the norm of its LCI result vector. Elementary flows with the highest intensities lead the direction of the vector; it is through these dimensions that the LCI result distinguished itself from the LCI result database.

Elementary flow pattern: the pattern of a LCI result refers to how the elementary flow intensities are distributed within a LCI result.

French extended abstract (résumé étendu)

Contexte et objectifs généraux

L'évolution de nos activités

Au XIXème siècle, la révolution thermo-industrielle a permis à une large partie de l'humanité de transformer radicalement son mode de vie et ses besoins. Principalement par l'exploitation du charbon, du pétrole et du gaz, la société industrielle s'est construite pour fournir une diversité de produits et de services qui améliorent (ou constituent une base utile pour l'amélioration) le bien-être de sa population, son éducation, sa mobilité, ses libertés, sa créativité et son bonheur. Face à cette situation idéalisée, le développement humain est aujourd'hui confronté à la fois à des ressources naturelles limitées (Meadows et al., 1972) et à une capacité d'assimilation limitée des grands cycles biogéochimiques (Hoekstra and Wiedmann, 2014). L'utilisation excessive d'énergie, des terres, de la fertilité des sols, de l'eau et autres matériaux, associée aux émissions anthropiques qui tendent à modifier les équilibres naturels actuels, ont engendré des défis environnementaux et sociaux majeurs. La pérennité de nos activités est questionnée face aux nombreux enjeux comme ceux identifiés par les Nations Unies à travers les 17 objectifs de développement durable des sociétés humaines (United Nations, 2015). Mesurer la pression des activités humaines sur l'environnement est alors nécessaire pour réduire notre empreinte environnementale. Une métrique est indispensable pour chercher à remplir ces objectifs de développement durable. Parmi les approches d'évaluation des impacts sur l'environnement, l'analyse du cycle de vie (ACV) est un outil normalisé (ISO, 2006a, 2006b) et reconnu internationalement.

L'Analyse du Cycle de Vie

L'ACV est une méthode dite « orientée produit » qui permet de quantifier les impacts marginaux potentiels d'un produit, d'un service ou d'un système sur l'ensemble de sa chaîne de valeurs (son cycle de vie). Cette analyse environnementale relève d'une approche multicritère en calculant des impacts tant sur l'épuisement des ressources naturelles (eau, énergie primaire…), sur la qualité des écosystèmes (eutrophisation, écotoxicité…) que sur la santé humaine (toxicité, particules…). L'ACV permet ainsi d'identifier les étapes d'un cycle de vie qui peuvent être améliorées dans le but de diminuer sa charge environnementale, tout en limitant les transferts de pollution vers une autre étape ou vers une autre problématique environnementale. Cette évaluation environnementale est réalisée sur la base de la fonction rendue par le produit, service ou système évalué. En comparant via l'ACV plusieurs systèmes qui remplissent la même fonction, l'ACV est un outil clé pour l'aide à la décision.

Le cadre méthodologique de l'ACV suit quatre grandes étapes : définition des objectifs et du champ d'étude, procédure d'inventaire des flux du cycle de vie, évaluation des impacts potentiels et interprétation. Ce travail de thèse se concentre sur les deux principales en reliant les résultats de l'inventaire et l'évaluation des impacts potentiels.

Pour obtenir un résultat d'Inventaire du Cycle de Vie (ICV), les flux de matières et d'énergies (les flux élémentaires), prélevés ou émis dans l'environnement, sont recensés et quantifiés depuis l'étape d'extraction des matières premières jusqu'au traitement du produit en fin de vie. Lors de la phase d'Évaluation de l'Impact du Cycle de Vie (ECVI), le résultat d'ICV est traduit sous forme d'indicateurs environnementaux sur un ensemble de catégories d'impact. Les flux élémentaires sont multipliés par des facteurs de caractérisation (FCs). En se basant sur une chaîne de causalités, ces FCs modélisent les conséquences de chaque flux vis-à-vis des problématiques environnementales.

Des résultats d'ICV déjà modélisés sont regroupés au sein de bases de données qui regroupent un nombre important d'activités humaines (environ 10,000 activités pour les bases les plus récentes). Celles-ci sont d'une grande aide pour les praticiens ACV en leur évitant de tout modéliser à chaque nouvelle étude : ils peuvent utiliser des résultats déjà obtenus pour de nombreux sous-systèmes (comme un mix de production électrique dans un pays donné ou un transport maritime par exemple).

Les catégories d'impact (les enjeux environnementaux) sont regroupées à travers des méthodes de calcul, une dizaine d'entre elles sont proposées par la littérature. Chaque méthode propose d'étudier les résultats d'ICV à travers un ensemble de 10 à 20 catégories d'impact. Les principales différences qui existent entre méthodes viennent des modèles de caractérisation des mécanismes environnementaux utilisés pour le calcul des FCs, des flux élémentaires pris en compte ou encore des différences d'échelles temporelles et spatiales considérées.

Sélection des méthodes d'impacts

Lors d'une étude ACV, le choix de la méthode de calcul et des catégories d'impact est primordial pour le praticien. Ce choix dépend de nombreux facteurs comme les exigences de la problématique de l'étude définie dans les objectifs, les recommandations internationales ou d'experts, ou encore les connaissances et les habitudes du praticien.

Le caractère holistique de l'ACV, qui a entraîné la production de nombreuses catégories d'impacts différentes, peut rendre difficile le choix de la méthode et des catégories d'impact à étudier. Ainsi, la sélection des méthodes de calcul et des catégories d'impact est tout d'abord réalisée lors de la phase de définition des objectifs et du champ d'étude, puis un approfondissement de certains résultats de catégories d'impact est effectué lors de l'interprétation. Afin de réduire le nombre de résultats de catégories d'impact à interpréter, différentes méthodes de sélection ont été développées comme ne considérer une différence entre les alternatives qu'à partir d'un certain seuil (ordre de grandeur de 20%), utiliser des valeurs de normalisation ou pondération, ou encore étudier les redondances observées entre résultats de catégories d'impact.

Objectif et organisation de la thèse

Ce travail de thèse propose de prendre en considération d'un point de vue mathématique les exigences de l'ISO par rapport à la sélection de catégories d'impact qui doivent « refléter un ensemble complet de problèmes environnementaux liés au système de produits étudié ». En bénéficiant d'une vision globale des tendances des flux élémentaires au sein d'une base de données de résultats d'ICV, la méthodologie développée permet d'évaluer, au sein d'un espace vectoriel standardisé, la pertinence relative du choix de la méthode de calcul et des catégories d'impact par rapport aux résultats d'ICV obtenus lors d'une ACV.

Le **Chapitre 2** présente le développement méthodologique d'un Indice de Représentativité (IR). Suite à une formalisation vectorielle de l'ACV, cette métrique est utilisée pour explorer les distances entre résultat d'ICV et méthodes de calcul au sein de l'espace vectoriel d'étude. L'adéquation des méthodes peut ainsi être comparée pour chaque résultat d'ICV.

En se basant sur l'IR, le **Chapitre 3** propose un outil de sélection de catégories d'impact au sein d'une méthode de calcul. Les liens entre l'IR global d'une méthode et l'ensemble des IRs des catégories d'impact de cette même méthode sont approfondis. Une analyse des dimensions, sur lesquelles chaque IR se base, a permis de déterminer des dimensions dites environnementalement critiques pour chaque catégorie d'impact.

Une analyse des résultats d'IRs est réalisée dans le **Chapitre 4**, en regroupant les résultats d'ICV par grands domaines d'activité. Ceci permet d'explorer la diversité de ces secteurs et de dégager des tendances dans leur représentation.

Le **Chapitre 5** applique cette méthodologie sur l'ACV d'une production de carburant à partir de macro-algue cellulosique. Ce cas d'étude se base sur l'inventaire obtenu dans le cadre du projet Green AlgOhol (ANR-14-CE05-0043) dans lequel s'inscrit cette thèse. L'enjeu est de contribuer à une démarche d'écoconception en apportant une information sur les critères regardés.

Les potentialités et des perspectives de l'approche sont enfin présentées au **Chapitre 6**.

Chapitre 2. Représentativité des méthodes de calcul d'impacts environnementaux au regard des résultats d'ICVs

Objectif du chapitre

Ce chapitre pose les fondements méthodologiques de la mesure de représentativité développée durant la thèse. Formalisant l'ACV avec un point de vue géométrique, l'IR est défini afin d'évaluer la part d'information des systèmes analysés représentée par les méthodes de calcul d'impact. L'IR est une mesure d'adéquation entre résultat d'ICV et méthodes d'impact, il n'apporte aucune information sur la validité scientifique des modèles mis en œuvre dans les méthodes.

Méthodes

L'interprétation géométrique de l'ACV permet de définir un espace vectoriel généré par les dimensions associées à chaque flux élémentaire d'une base de données. Chaque résultat d'ICV peut être localisé au sein de cet espace. De la même façon, les catégories d'impact d'une méthode de calcul sont localisées grâce à leur FCs. Le calcul des résultats d'impacts est alors assimilé à un produit vectoriel entre le vecteur de résultat d'ICV et chaque vecteur de catégorie d'impact.

Les directions des résultats d'ICVs et des catégories d'impact sont déterminées par les flux élémentaires et les FCs. Afin de s'affranchir des normes de chaque vecteur, l'IR se base sur la mesure du cosinus de l'angle formé entre le résultat d'ICV et chaque catégorie d'impact ou le sous espace vectoriel généré par l'ensemble des catégories. Ainsi, un fort IR révèlera une forte proximité entre ces vecteurs. Ce chapitre se focalise sur les IRs globaux des méthodes de calcul et non les IRs des catégories d'impact.

Les expressions mathématiques de la métrique développée pour un résultat d'ICV $\mathbf{g}_i$ et une catégorie d'impact $\mathbf{q}_j$ puis une méthode de calcul Q sont alors :

$$RI(\mathbf{q}_j, \mathbf{g}_i) = \left|\cos(\alpha_{j,i})\right| = \left|\frac{\langle \mathbf{q}_j, \mathbf{g}_i \rangle}{\|\mathbf{q}_j\| \cdot \|\mathbf{g}_i\|}\right| \qquad RI(\mathbf{Q}, \mathbf{g}_i) = \sqrt{1 - \left(\frac{\|\mathbf{g}_i - \mathbf{g}_{i,Q}\|}{\|\mathbf{g}_i\|}\right)^2}$$

Où $\alpha_{j,i}$ est l'angle entre les vecteurs $\mathbf{g}_i$ et $\mathbf{q}_j$; et $\mathbf{g}_{i,Q}$ le projeté orthogonal de $\mathbf{g}_i$ sur l'hyperplan généré par les catégories d'impact de $\mathbf{Q}$.

Etant donnée la diversité des unités et des ordres de grandeur des flux élémentaires au sein d'une base de données telle qu'ecoinvent 3.1 (Wernet et al., 2016), une standardisation des flux d'inventaires est nécessaire afin d'harmoniser les plages des valeurs des flux élémentaires sur chaque dimension. Ces plages de valeurs étant sur des échelles logarithmiques nettement différentes, leurs moyennes géométriques sont utilisées pour diviser chaque flux de chaque inventaire. De même, les FCs sont standardisés en les multipliant par ces moyennes géométriques. Cette standardisation permet de contextualiser les résultats d'ICV et les catégories d'impact par rapport à la base de données étudiée.

Résultats

La méthodologie est testée sur quatre mix électriques issus de la base de données ecoinvent 3.1 pour 18 méthodes de calcul. Les résultats ont mis en évidence des différences de représentativité entre les méthodes de calcul pour chacun des inventaires étudiés (Figure 1). Cela montre l'intérêt potentiel de l'utilisation d'un tel indice pour discuter de l'adéquation de la méthode de calcul choisie pour un inventaire donné.

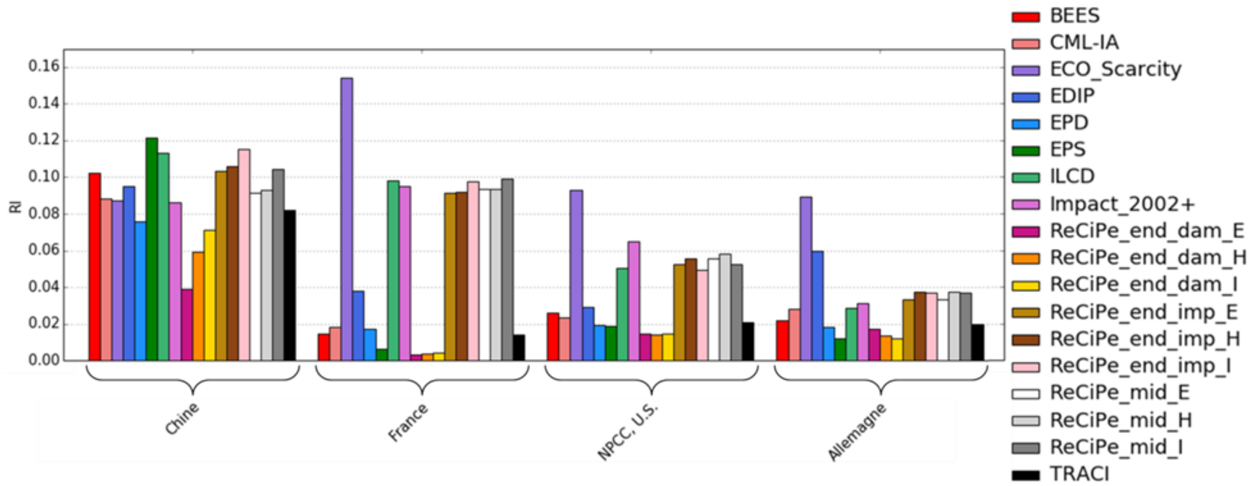


Figure 1. IRs globaux des méthodes de calcul pour les quatre mix électriques

Lors d'une comparaison de plusieurs résultats d'ICV avec une méthode donnée, ces indices montrent les potentielles différences de représentativité. Une méthode peut être adéquate pour l'un des résultats d'ICV mais ne pas représenter les principales problématiques environnementales pour un autre.

Une courte analyse des IRs des catégories d'impact de la méthode ReCiPe midpoint Individualiste est finalement présentée pour le mix chinois et français. Avec des IRs similaires de méthode, cette analyse montre les disparités qui existent sur les IRs des catégories d'impact. Ces IRs de catégories d'impact font l'objet d'une étude plus approfondie dans le Chapitre 3.

Le Chapitre 2 a fait l'objet d'un article publié dans la revue Science of the Total Environment, Volume 621, Avril 2018, Pages 1264–1271 (https://doi.org/10.1016/j.scitotenv.2017.10.102)

Chapitre 3. Un outil d'aide à la sélection des catégories d'impact lors d'une ACV

Objectif du chapitre

Le Chapitre 2 ayant présenté l'IR et l'ayant appliqué aux méthodes de calcul, le Chapitre 3 propose l'utilisation de cette métrique pour aider au choix des résultats de catégories d'impact pertinents dans une méthode sur lesquels approfondir l'interprétation d'une ACV. L'IR est ici un outil d'aide à la réduction du nombre de catégories d'impact à étudier afin de faciliter la prise de décision. Un ensemble de scripts, écrit en langage Python, est proposé au téléchargement via un dépôt en ligne (DOI: 10.5281/zenodo.1068914) pour permettre le calcul de l'IR de méthode et de catégories d'impacts.

L'étude des IRs des catégories d'impact par rapport à l'IR global d'une méthode a mis en évidence que les corrélations entre catégories d'impact standardisées d'une même méthode peuvent amener une sur-représentativité ou une sous-représentativité des catégories d'impact. Pour résoudre ces problèmes de représentativité, un algorithme de décorrélation des IRs a été développé.

Méthodes

Les liens entre l'IR global d'une méthode et l'ensemble des IRs des catégories d'impact de cette même méthode sont ici approfondis. En effet, du fait d'une non orthogonalité parfaite des catégories standardisées, il peut exister une différence entre la somme des carrés des IRs de catégories d'impact et le carré de l'IR global de la méthode de calcul. Un algorithme de décorrélation des IRs de catégories d'impact est ainsi proposé afin que les valeurs obtenues correspondent à l'IR global de la méthode utilisée.

Cet algorithme est tout d'abord appliqué à deux mix électriques (Allemagne et Chine) issus de la base de données ecoinvent 3.1 pour la méthode de calcul de l'ILCD. Les IRs obtenus sont alors mis en relation avec les résultats d'ACV de ces résultats d'ICVs.

En considérant l'ensemble des résultats d'ICV de la base de données, une analyse des distributions des résultats des IRs de catégories d'impact est réalisée. Les corrections des IRs obtenues par l'algorithme de décorrélation sont aussi analysées sur tous ces résultats d'ICVs. Ce chapitre propose finalement une interprétation des indices en s'appuyant sur les valeurs des flux élémentaires et des FCs qui fournissent la plus grande partie de la valeur des IRs.

Résultats

Les résultats du cas d'étude de ce chapitre ont montré que le mix chinois est mieux représenté par l'ILCD et que les problématiques environnementales mises en avant par les IRs sont pour la plupart différentes entre les deux résultats d'ICVs (Figure 2). En effet, le mix chinois obtient des IRs élevés pour les particules fines, l'acidification, la formation d'ozone photochimique, le changement climatique et l'eutrophisation terrestre. Concernant le mix électrique allemand, les catégories d'impact sur lesquelles se concentrer sont les radiations ionisantes (HH), l'eutrophisation des eaux douces, le changement climatique, l'utilisation des ressources en eau et la toxicité humaine (hors cancers). L'utilisation des IRs permet de guider le praticien sur les principales catégories d'impact à interpréter et de nuancer des résultats obtenus sur l'ensemble des catégories de la méthode.

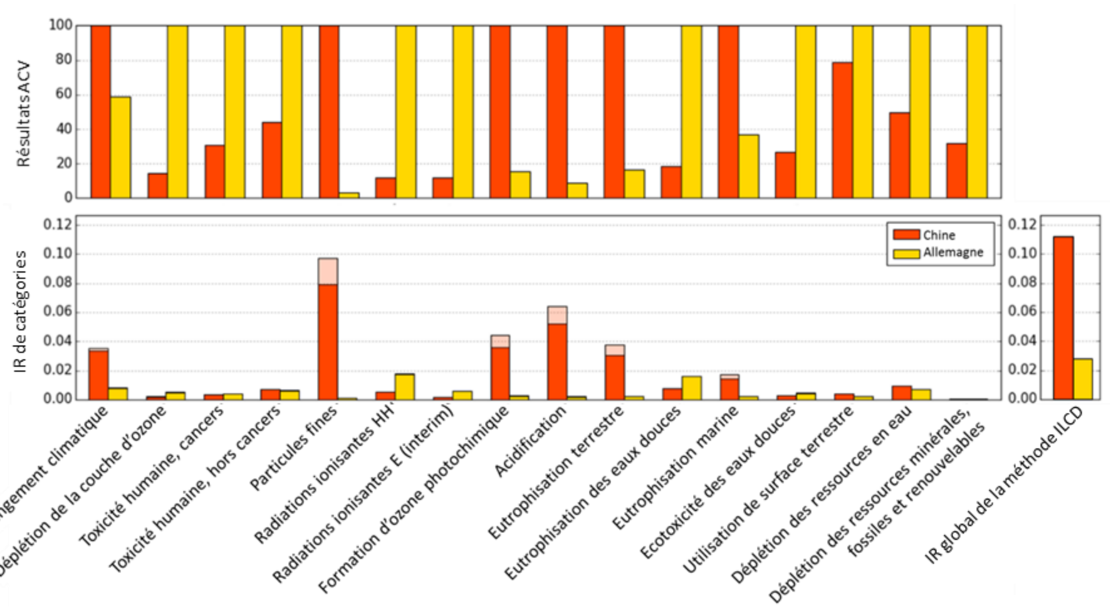


Figure 2. Résultats d'ACV et d'IRs des mix de production électrique chinois et allemand. Les écarts entre les IRs originaux et décorrélés (couleurs franches) sont représentés par des couleurs pastel.

L'algorithme de décorrélation des catégories n'entraîne pas de modifications des conclusions obtenues sur les IRs originaux. La détermination des dimensions qui soutiennent les valeurs des IRs a permis d'apporter à ces résultats d'intéressantes discussions complémentaires.

Sur l'ensemble des résultats d'ICV de la base de données, l'analyse des dimensions représentatives a mis en évidence que ce sont principalement les dimensions ayant des FCs importants, et non les flux élémentaires majoritaires, qui sont le plus fréquemment à l'origine de la valeur des IRs. Ces dimensions seraient des dimensions critiques d'un point de vue environnemental pour la base de données étudiée. Grâce à la prise en compte des tendances des flux élémentaires sur toute la base de données, les catégories les plus représentatives des intensités d'un résultat d'ICV sont donc les plus pertinentes à étudier.

Le Chapitre 2 a fait l'objet d'un article publié dans la revue Science of the Total Environment, Volume 658, Mars 2019, Pages 768–776 (https://doi.org/10.1016/j.scitotenv.2018.12.194)

Chapitre 4. Représentativité des catégories d'impact en fonction des domaines d'activité

Objectif du chapitre

Ce chapitre se propose d'explorer les tendances des résultats d'IRs en regroupant les résultats d'ICV par grands domaines d'activité. Cette étude permet de tester comment cette métrique met en avant des méthodes d'impacts (et des catégories d'impact) en fonction des domaines d'activités où les inventaires se placent.

Méthodes

En se basant sur la classification internationale de normalisation en industrie, pour toutes les branches d'activité économique (International Standard Industrial Classification, ISIC), 9 622 résultats d'ICV provenant de quatorze grands domaines d'activité ont pu être étudiés. Les IRs sont étudiés à travers leur distribution (médiane et interquartile) pour les différentes méthodes d'impacts et leurs catégories.

Résultats

Les distributions des IRs de la méthode de calcul de l'ILCD montrent des différences entre domaines d'activités (Figure 3). Cette méthode permet de bien représenter les résultats d'ICV des domaines d'activités de la production de machines et matériels de transport, de la production d'électricité ou encore de la construction. Par contre, le domaine de l'agriculture et de la sylviculture, par exemple, ne semble pas être globalement bien représenté.

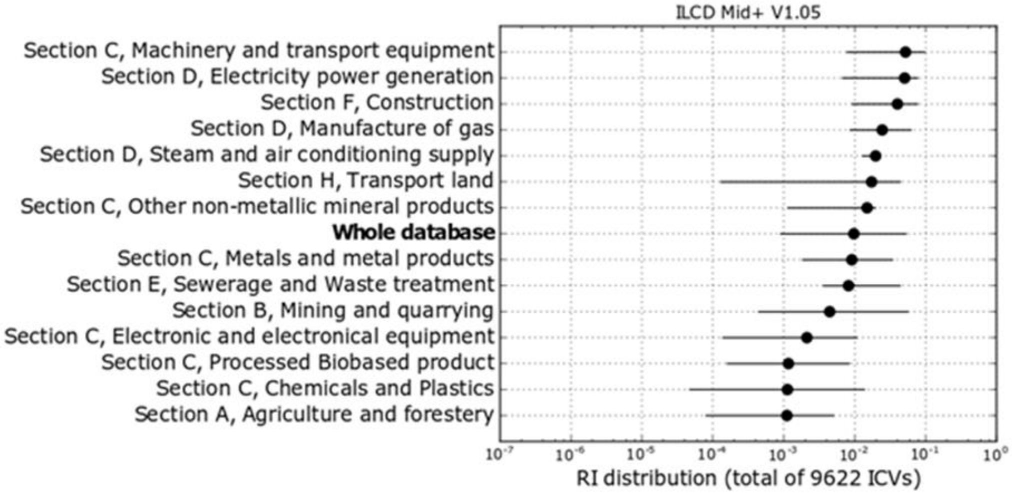


Figure 3. Distributions des IRs globaux de la méthode de calcul de l'ILCD en fonction des domaines d'activité

L'analyse des distributions de IRs des 16 catégories d'impacts de l'ILCD a ensuite permis de faire ressortir des catégories plus ou moins pertinentes par domaine d'activité. Le changement climatique, la formation d'ozone photochimique et l'acidification des milieux sont les catégories les plus représentatives pour le domaine de la production d'électricité tandis que l'utilisation de surface terrestre et les catégories d'eutrophisation marine et terrestre sont celles sur lesquelles approfondir les résultats d'ACV de produits issus de l'agriculture et de la sylviculture.

Ce chapitre a ainsi permis d'obtenir une vision globale des résultats possibles de la méthodologie développée en séparant les résultats d'ICV suivant des groupes d'activité homogènes. Ces résultats pourraient être une base pour fournir des recommandations de catégories d'impact pertinentes par domaine d'activité.

Chapitre 5. Application sur l'ACV d'une production de carburant à partir de macro-algue cellulosique

Objectif du chapitre

Ce dernier chapitre du corps de la thèse applique l'IR sur l'ACV d'une production de carburant à partir de macro-algue cellulosique. Ce cas d'étude se base sur l'inventaire obtenu dans le cadre du projet ANR Green AlgOhol.

Méthodes

Les IRs de différentes méthodes et de leurs catégories respectives sont calculés sur le résultat d'ICV ainsi que sur quatre sous-systèmes de la chaîne de valeurs. L'ACV réalisée étudie la chaîne de valeurs présentée en Figure 4 à travers l'unité fonctionnelle « parcourir 100 km dans une voiture de tourisme de moyenne taille ».

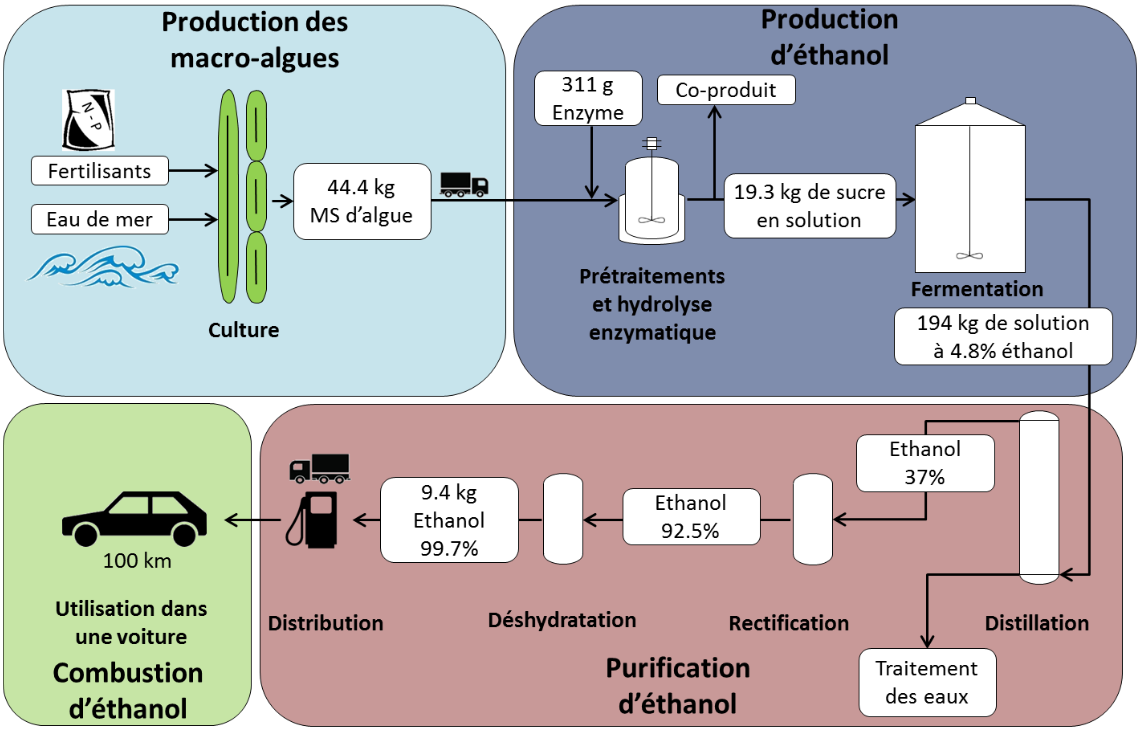


Figure 4. Représentation schématique de la chaîne de valeurs étudiée

Le travail d'inventaire se base sur des données de laboratoire obtenues dans le cadre du projet, de simulations de productions industrielles (logiciel Aspen) et issues de la littérature. La modélisation de l'ICV utilise la base de données ecoinvent 3.1. La méthode de calcul utilisée pour déterminer les impacts potentiels est la méthode de l'ILCD. Une analyse des contributions environnementales est alors menée.

Résultats

L'étude des impacts montre que la production des algues est la principale étape contributrice pour 13 des 15 catégories d'impact. C'est notamment à cause de l'électricité utilisée pour mettre en mouvement l'eau dans les bassins et la construction même des bassins que ce système impacte sur l'environnement. Les autres étapes de la chaîne de valeurs affectent les catégories sans dépasser 20% de l'impact global du système, excepté pour l'étape de combustion (liée à la construction du véhicule) dont la part monte à plus de 30% pour les toxicités et l'écotoxicité, l'eutrophisation de l'eau douce et l'utilisation de ressources naturelles.

Le calcul des IRs de l'ILCD a permis de mettre en évidence la forte représentativité des radiations ionisantes, de l'utilisation de surface terrestre et de ressources naturelles. L'obtention des IRs des quatre sous-systèmes a montré qu'étendre l'analyse à cinq autres catégories d'impacts supplémentaires permettrait d'avoir une meilleure représentativité de l'ensemble du résultat d'ICV. Les trois premiers sous-systèmes, la production de macro-algues et la production et la purification de l'éthanol, obtiennent des IRs plus élevés que l'ensemble de résultats d'ICV. La production d'éthanol a l'IR le plus élevé qui se rapproche de la médiane des IRs de la base de données (chapitre 4). Si un système global peut être mal représenté par une méthode d'évaluation, les sous-parties, considérées séparément, peuvent être bien appréhendées. La combustion de l'éthanol reste mal représentée par l'ILCD avec un IR du même ordre de grandeur que celui de l'ensemble.

La production des macro-algues est la principale étape contributive de l'ensemble du système pour la plupart des impacts, mais ce n'est pas l'étape la mieux représentée par l'ILCD. Ceci souligne la nécessité de focaliser l'attention dans cette étape pour l'amélioration du système et de l'évaluation.

Finalement, en étendant l'analyse des IRs à d'autres méthodes de calcul et leurs catégories d'impacts, l'ILCD n'était pas forcement la méthode la plus représentative de ce résultat d'ICV. En effet, à travers des catégories comme par exemple l'utilisation de surface urbaine ou la comptabilisation des émissions de pesticides, des méthodes comme ReCiPe ou Ecological scarcity pourraient amener une représentation plus précise des flux élémentaires problématiques de l'inventaire au regard de la base de données.

Chapitre 6. Discussion et conclusion générale

L'objectif principal de la thèse était le développement d'une métrique permettant d'évaluer la pertinence du choix d'une méthode de calcul et des catégories d'impact associées. Ce travail a ainsi abouti au développement d'un indice de représentativité où l'ACV est abordée comme une projection géométrique.

En bénéficiant de l'étude globale de bases de données de résultats d'ICV, la mise en perspective de chaque résultat d'ICV et la contextualisation des catégories d'impact par rapport à cette base ont permis de considérer d'une manière innovante la sélection d'indicateurs environnementaux. Ce travail de thèse ouvre plusieurs perspectives.

Concernant la standardisation utilisée et du fait de la constitution même des bases de données de résultats d'ICV, la surreprésentation de certains domaines d'activité (par exemple, ecoinvent possède plus de 2788 résultats d'ICV de production d'électricité mais ne rassemble que 280 résultats d'ICV d'extraction minière) peut orienter les tendances des flux élémentaires vers ces mêmes domaines. L'utilisation de bases de données « input-output » pourrait fournir des valeurs de standardisation qui reflèteraient les tendances d'émissions du « monde réel » avec une meilleure fidélité. Cela permettrait de prendre en compte les importances relatives des secteurs d'activité entre eux, en fonction des flux monétaires échangés.

Le partage d'informations surreprésentées ou sous-représentées par l'algorithme de décorrélation du Chapitre 3 prend en compte les corrélations entre les vecteurs de catégories d'impact puis les valeurs des IRs originaux. Cette procédure peut entrainer des résultats où des IRs sont modifiés sans que les dimensions associées qui engendrent ces problèmes de représentativité ne soient celles sur lesquelles les vecteurs de catégories sont corrélés. Une perspective intéressante serait donc de baser la répartition de l'information redondante de représentativité sur l'étude des dimensions et non des catégories d'impact.

La régionalisation et l'étude de la variabilité en ACV sont des domaines qui n'ont pas été abordés au regard de la méthodologie développée. Le détail des données au niveau régional va augmenter le nombre de dimensions au sein des bases de données, ce qui nécessitera des adaptations de la méthodologie des IRs. Les liens entre la variabilité en ACV et la variabilité au niveau des IRs devront aussi être étudiés en détail.

Enfin, en élargissant le calcul des IRs sur l'ensemble des catégories d'impact mises à disposition par les méthodes de calcul, la création de « méthodes composites » qui concentrent des indicateurs environnementaux pertinents au regard du résultat de l'ICV pourrait être une aide précieuse pour un praticien menant une étude d'écoconception.

L'un des principaux atouts de l'approche ACV vient de la structuration qu'elle apporte. Les enjeux environnementaux d'une activité humaine sont abordés à travers deux aspects : les chaînes de valeurs (ICV) sont modélisées par les praticiens et les développeurs de méthodes fournissent des outils d'évaluation (méthodes ACVI) qui modélisent des mécanismes environnementaux. Les travaux présentés dans cette thèse contribuent à une meilleure cohérence entre ces deux étapes afin de contribuer à une meilleure pertinence et efficacité des évaluations environnementales.

Chapter 1: General introduction

Contents of Chapter 1

This first chapter presents the context of the theoretical development of the thesis. A bibliographical review addresses the selection of LCIA method and impact category in LCA. Then, it introduces the research question, the objectives and the general structure of the thesis.

1.1. Context

The thermo-industrial revolution that broke out in the XIXth century has brought countless positive transformations in the way of life and needs of a large part of mankind. Mainly due to coal, oil and gas exploitation, our modern industrialized society can provide a huge diversity of products and services that support, or set a valuable background for, the welfare, the education, the mobility, the freedom ,the creativity and the happiness of its own people. However, human development is nowadays facing both limited natural resources (Meadows et al., 1972) and limited assimilation capacity of the major biogeochemical cycles (Hoekstra and Wiedmann, 2014). Overexploitation of energy, land, soil fertility, water and material combined with anthropic emissions that tend to modify current natural balances rise major environmental and social challenges. This led the United Nations to adopt 17 Sustainable Development Goals in 2015 for human societies (see Figure 5, United Nations, 2015). Apprehending and measuring the human pressure on the environment is then necessary to reduce humanity's environmental footprint if we want to achieve some of the Sustainable Development Goals one day. Among environmental impact assessment approaches, the Life Cycle Assessment (LCA) framework is one of the most suitable one.

Figure 5. The sustainable development goals to end poverty, protect the planet and ensure prosperity for all (United Nations, 2015)

1.2. Life Cycle Assessment

LCA is a standardized and internationally recognized approach for environmental evaluation (ISO, 2006a, 2006b). This decision-making tool quantifies the potential environmental marginal impacts of a product or a service within all its values chain. LCA is a multi-criteria assessment that covers the potential impacts of the studied system on a set of environmental impact categories: from natural resource consumptions (energy, water, land…), as well as on ecosystem quality (eutrophication, eco-toxicity…) and human health (particulate matter, toxicity…). LCA allows identifying the life cycle stages that need to be focused on, i.e. the environmental "hot-spot", to mitigate the environmental burden of the whole system. Having a holistic point of view of the impacts over the whole system, LCA can prevent burden shifting from an environmental impact category to another, or from a life cycle stage to another. This assessment is realized on the basis of a functional unit, that is associated with a measurable referenced flow, and that reflects the function(s) fulfilled by the product(s) or service(s): comparison of systems that have the same functional unit is then possible.

In the four-step framework of LCA, beginning with the goal and scope and ending with the interpretation, the two main steps on which the presented work will focus on are the Life Cycle Inventory procedure (LCI) and the Life Cycle Impact Assessment (LCIA) (see Figure 6). The LCI procedure describes the studied production system throughout its values chain (from raw material extraction, through materials processing, production, distribution and use stages, to waste management, e.g. disposal or recycling) and quantifies within a LCI result all emission flows to the environment as well as all resource consumption flows (all defined as elementary flows). At the LCIA level, elementary flows are translated in terms of category indicators. Elementary flows are multiplied by a Characterization Factor (CF), quantifying to what extend they contribute to a given environmental impact category, based on cause-effect chains, also called environmental impact pathways. These impact categories (at midpoint level) can be assessed through their damages (at endpoint level) and further aggregated into three area of protection: Resources, Ecosystems quality and Human health.

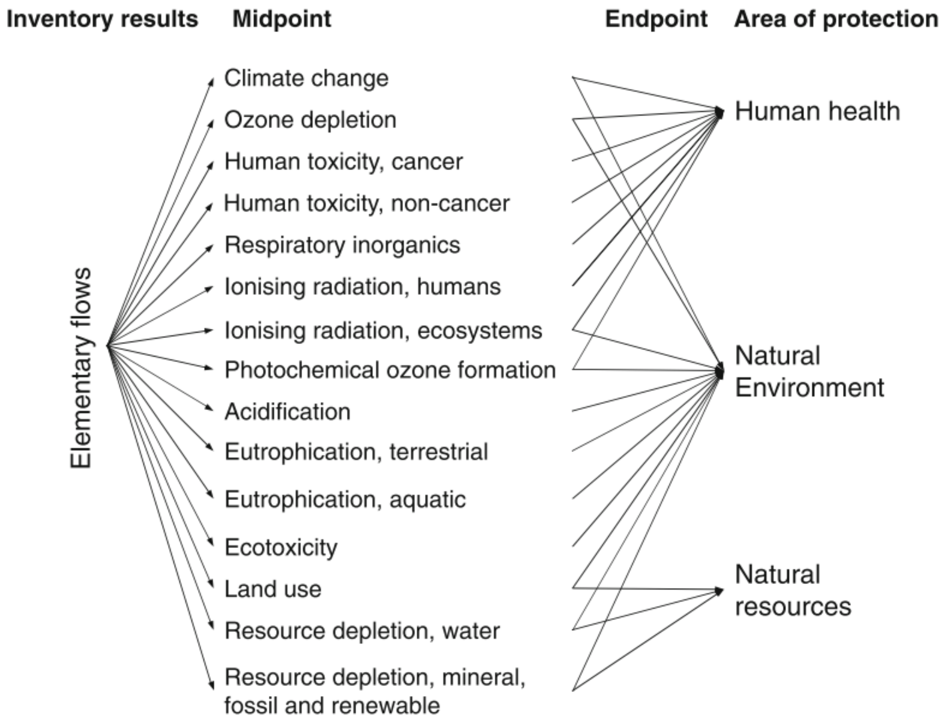


Figure 6. Framework of the ILCD LCIA method, linking elementary flows to midpoint and endpoint indicators, extracted from Hauschild et al. (2013)

1.3. Data structure in LCA

LCA is a framework that allows translating elementary flows from a human activity into a reduced number of scores that each has an environmental meaning. LCA handles datasets that model human activities (LCI results and its elementary flows) and model environmental mechanisms (impact category and its CF).

1.3.1. LCI results and LCI results database

Sets of LCI results are gathered within LCI results databases. Each stage of a Life Cycle is modelled by a structure called “Unitary process” (see Figure 7). It inventories the technological inputs and outputs (the technology matrix) and the elementary flows (the intervention matrix) of that specific stage. The technology matrix links all unitary process of a LCI database between each other: it represents the human activities network. An aggregated LCI (“System process”) consists in the quantification of all elementary flows over an entire process tree. It results from the computation of a final demand vector (product), the technology matrix and the intervention matrix (Heijungs and Suh, 2002). Both unitary and system process databases (the second type is obtained from the first one) can be used depending on the aim of each LCA study. A system process database can be seen as a set of aggregated LCI results representing all modelled human activities that belong to numerous fields of activity (for example: agriculture and forestry, electricity power generation or machinery and transport equipment…).

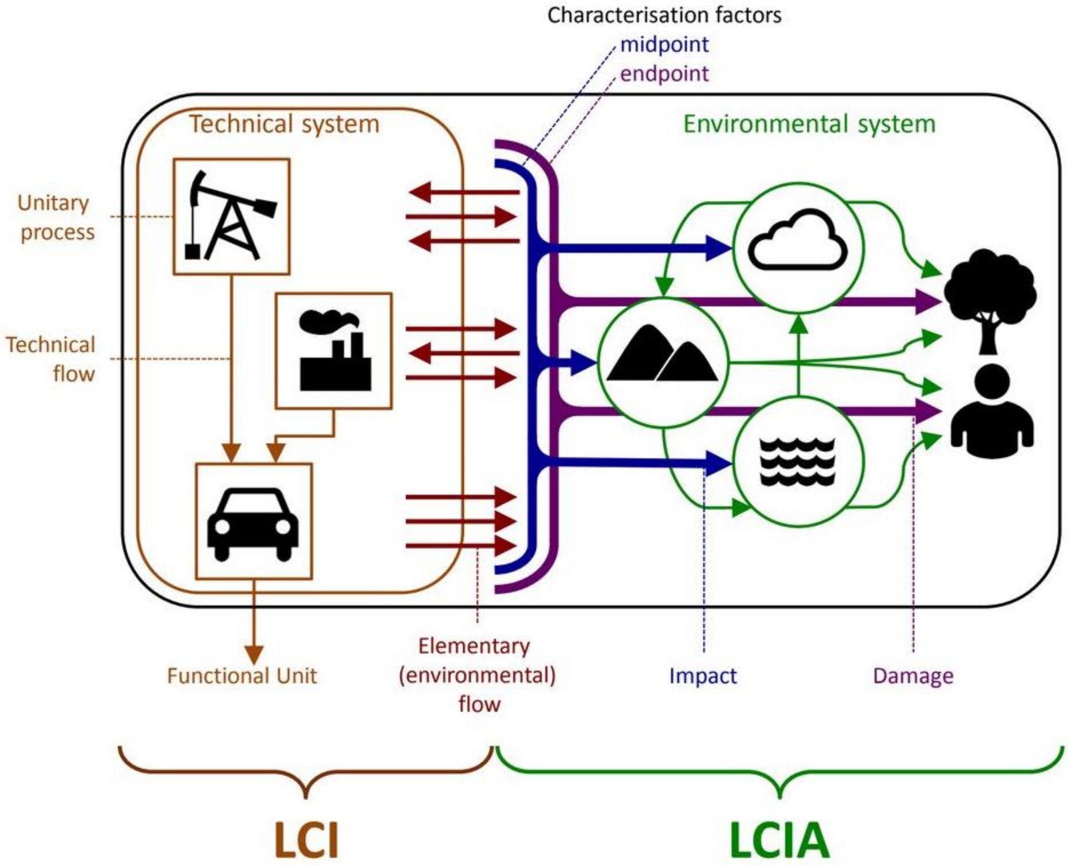


Figure 7. Technical and environmental system in LCA

Emission flows to the environment and resource consumption flows are the elementary flows of a LCI result. They reflect the intervention of human activities with the environment. Each elementary flow is expressed within an emission or an extraction unit that is common for the entire LCI result database. A dimension is defined by its unit, an environmental compartment and a sub-compartment where the substance is emitted: the fossil CO_2 emission (substance), kg (unit), to air (compartment), urban air close to ground (sub-compartment).

The number of dimensions observed in a LCI result database depends on the environmental interventions took into account by developers. Each LCI result is a vector that can be localized in a linear space by the value of its elementary flows taken on each dimension of the database.

1.3.2. Impact categories and LCIA methods

The impact categories (at midpoint, endpoint and damage level) are the criteria used to characterize, assess and compare production systems. For each impact category (e.g. climate change, particulate matter or resource depletion…), a category indicator is defined (e.g. CO2 equivalent, PM2.5 equivalent or antimony equivalent…). Elementary flows of a LCI result are converted into a corresponding amount of the category indicator by means of CFs: CF units are expressed in indicator unit equivalents per unit of elementary flow. CF values result from the modelling of environmental mechanisms. For a given environmental mechanism, all related CFs form the characterization model of its corresponding impact category. The environmental relevance and the scientific validity of the characterization models are constantly challenged to update the best practice (Bare and Gloria, 2006; Hauschild et al., 2013; Jolliet et al., 2018; Rack et al., 2013; Udo de Haes et al., 1999).

LCIA methods are associated to ready-to-use sets of impact categories (EC-JRC, 2010a; Hauschild et al., 2013). Quite a few impact categories and LCIA methods are now available for LCIA. Figure 8 provides an overview of major LCIA methods published since 2000: each LCIA method is composed of 10 to 20 different impact categories.

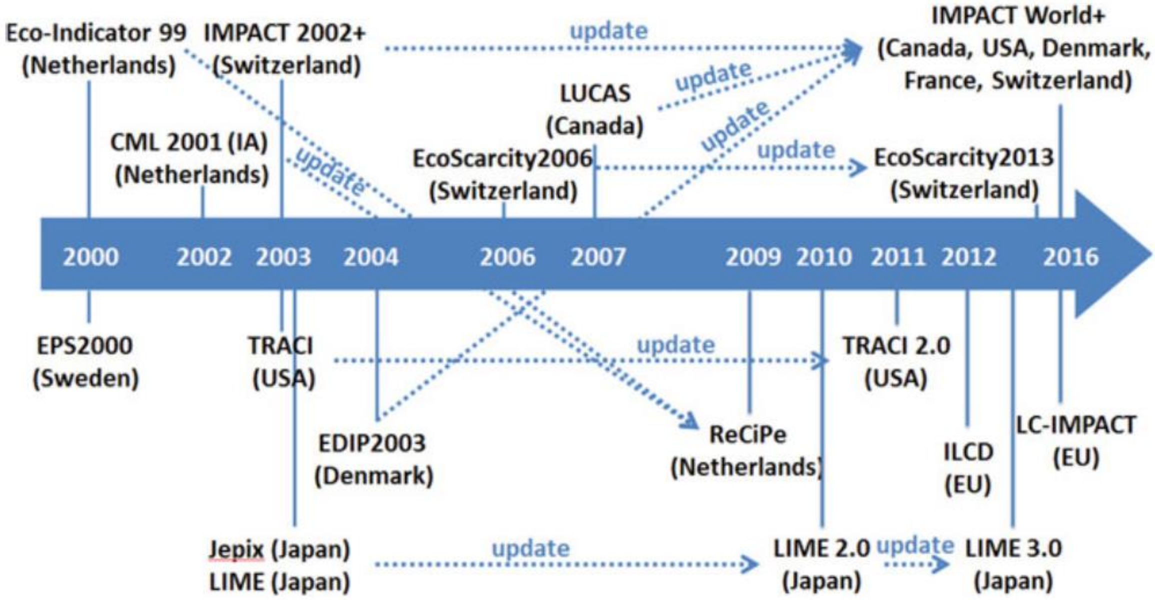


Figure 8. LCIA methods published since 2000 (country/region of origin in brackets), extracted from Rosenbaum (2017)

1.4. Selection of LCIA methods and impact categories

1.4.1. During the goal and scope definition phase

During the goal and scope definition phase, the selection of a LCIA method and impact categories is one of the crucial steps for LCA practitioners. They often choose a LCIA method (or a subset of impact category proposed by a LCIA method) according to (i) existing guidelines bearing the latest update of LCIA methods, (ii) the context and the decision maker needs defined in the goal and scope definition phase, (iii) the modelling choice of the impact categories belonging to a method (the intended purpose, the problem or damage-oriented approach, the covered impacts, the regional and temporal validity of the method…) but also (iv) the habits and the expertise of the LCA practitioner (EC-JRC, 2011; Guinée, 2015; ISO, 2006a, 2006b; Rosenbaum, 2017).

Concerning the selection of impact categories, the main requirements addressed by the ISO are:

- “the selection […] shall reflect a comprehensive set of environmental issues related to the product system being studied taking the goal and scope into consideration”
- “Value-choices and assumptions made during the selection […] should be minimized”

For LCA practitioners, the selection has been facilitate by the development of ready-to-use default lists of impact categories (i.e. the LCIA methods presented in Figure 8) (Guinée, 2015). Differences between these LCIA methods are due to the modelling choice of the environmental issues, the substance coverage, the relative ranking of the reference substance or are due to different spatial or time scales (Owsianiak et al., 2014). Traditionally, midpoint methods have been defined by their focus on the following five impact categories: stratospheric ozone depletion, global warming, acidification, eutrophication, and smog formation (Bare and Gloria, 2006). Other environmental concerns complete LCIA methods to up to 20 impact categories, as for example: toxicity categories, land occupation, pesticides into soil, energy resources, ionizing radiation...

Following the aim of being holistic, such large sets of impact categories can however challenge the LCIA method and impact categories selection and subsequently the efficiency of environmental regulation (as product eco-design, decision making or environmental labelling) (Steinmann et al., 2016). Guinée (2015) suggests that “it might be useful to distinguish between different types of default lists per specific sector”. Paying high attention to impact categories consistency and double counting, relevant impact categories could also come from different LCIA methods (Rosenbaum, 2017).

1.4.2. During the result interpretation phase

In addition to the selection of a LCIA method and impact categories during the goal and scope definition stage, a focus on a few impact categories can be carried out on LCIA results. The following paragraphs propose an overview of practical procedures that select the LCIA results that are worthwhile focusing on. These procedures determine the relevance from: (i) clear environmental distinctions between alternatives, (ii) external valuations or (iii) from redundancies between impact category results.

In comparative LCA and following the LCIA step, impact categories exclusion from interpretation (i) is sometimes carried out based on an empirical threshold value applied on the LCIA result differences: for instance, no clear conclusions can be done from LCIA results with less than 20% difference for a human toxicity indicator. By quantifying uncertainties, exploration of the relative importance of impact categories through the magnitude of differences between LCIA results can lead to promising tools in comparative LCA (Mendoza Beltran et al., 2018).

Within the ISO recommendation, existing practices for normalization and weighting (ii) use external valuation of impact categories that might guide LCA practitioners on a reduce subset of LCIA results to interpret. Valuation factors allow aggregating or comparing impact category results. Other weighting procedures are currently under development. On the basis of decision makers' preferences, surveys of public opinion, willingness to pay (implying monetarization of environmental issues) and expert’s knowledges, the relative importance of impact categories (i.e. weighting) is also explored using Multi-Criteria Decision Analysis (MCDA) and Linear Programming. However, all these procedures might be criticized due to the subjectivity of the weighting, inconsistency of monetarization approaches and safeguard subjects (Cortés-Borda et al., 2013; Prado-Lopez et al., 2014).

Other studies tackle this problem through redundancies (iii) that can be observed within LCIA results on specific case studies (few numbers of LCI results with the same functional unit). Using Principal Component Analysis (PCA) combined with uncertainty analysis or multi-objective optimization, these studies reveal impact category results relationships that lead to impact category grouping (Basson and Petrie, 2007; Bava et al., 2014; Chen et al., 2015; De Saxcé et al., 2014; Mouron et al., 2006; Pozo et al., 2012).

In the same context but applied on large sets of LCI results, Steinmann et al. (2016) proposed a procedure using PCA over a large range of products and LCIA methods (all the LCIA results of 135 impact categories for 976 LCI results from ecoinvent database 3.1) to select the impact categories explaining the major part of the variance in the product ranking. Other studies that apply multivariate statistical analysis or multi-linear regression on LCIA results of LCI results from different fields of activity focus on revealing 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, and then focus the interpretation on this reduce set of selected impact categories.

1.5. Objectives

We saw that the selection of worthwhile impact categories is carried out at two different stages of the LCA framework: the goal and scope definition phase and the LCIA results interpretation. The present work tends to take into consideration the ISO requirement of having a "comprehensive set of environmental issues related to the product system" with a mathematical point of view. LCI results databases provide a huge compilation of human activities and LCIA methods provide a wide diversity of potential environmental indicator. With the general aim of improving the selection procedure of LCIA methods and impact categories by analysing LCI database, the research question of the thesis is:

By exploring LCI results through their standardized elementary flow trends, is it possible to assess by a systematic approach the relative relevance of LCIA methods and their respective impact categories for LCA studies?

The Figure 9 presents the global structure of the thesis. After the introduction (**Chapter 1**), the **Chapter 2** defines and presents the theoretical development of the Representativeness Index (RI), established for the first time in this thesis. RI is a proximity measurement developed to explore, within a standardized vector space, the relationships between LCI results and LCIA methods through an angular distance. Within the standardized vector space, the representativeness can then be defined as the similarity between the LCI result vector and the impact category vector through the environmentally concerning dimensions. The relative adequacy of LCIA methods for LCI results is then analyzed.

Chapter 3 proposes a tool based on the RI methodology to guide impact categories selection for LCA studies. The links between the global RIs of LCIA methods, the RIs of their impact categories and the dimensions that support RI values are examined.

Chapter 4 analyses RI results among large sets of LCI results based on fields of activity. We explore if the RI methodology puts forward distinct LCIA methods and environmental issues while analysing datasets based on subtypes of products and activities.

Chapter 5 applies the RI methodology on the LCA of the production of biofuel from cellulosic macro-algae. First, an inventory of the system designed in the Green AlgOhol project is presented and a contribution analyses is carried out with the ILCD method. For the ILCD method, RIs of the whole system and sub-parts of the values chain are analyzed. A screening of classic LCIA methods and their impact categories is performed through their RIs.

Finally, a discussion about the scientific and practical relevance of the main outcomes of the thesis, along with future research perspectives to address their identified shortcomings, is provided in **Chapter 6**.

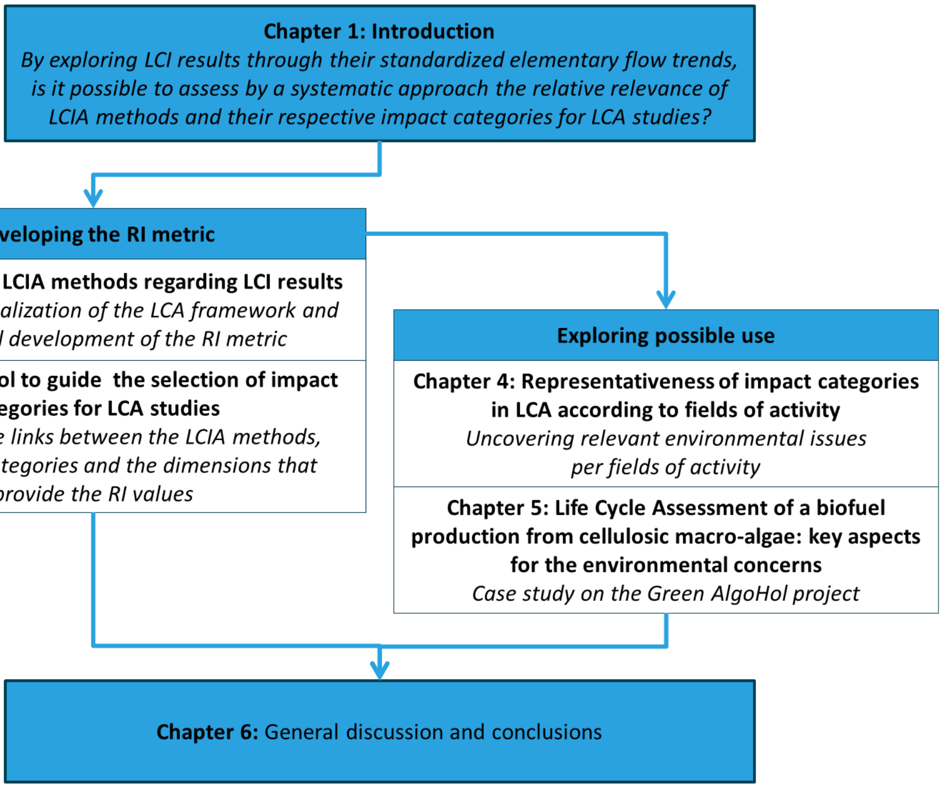


Figure 9. Structure of the thesis

Chapter 2: Representativeness of environmental impact assessment methods regarding Life Cycle Inventory results

---

Contents of Chapter 2

This chapter presents the theoretical development of the Representativeness Index. A geometric formalization of the LCA framework is proposed and the proximity measurement, on which the PhD work is based to explore the relationships between LCI results and LCIA methods, is defined. The relative adequacy of classic LCIA methods for four electricity mix production LCIs is analyzed.

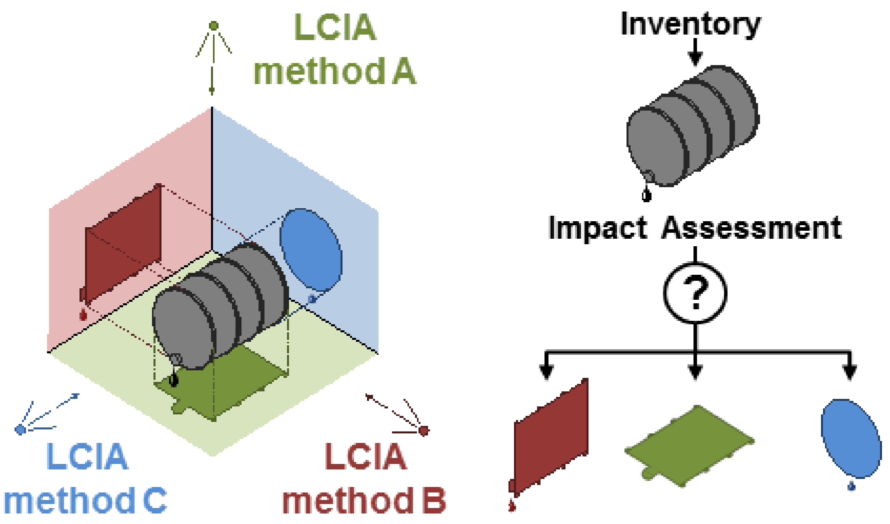


Figure 10. Graphical abstract of Chapter 2

2.1. Introduction

The LCA methodology provides a standardized and commonly used framework to quantify the environmental impacts of human activities (ISO, 2006b, 2006a). In the four-step framework of the LCA, beginning with the goal and scope and ending with the interpretation, the main steps are the Life Cycle Inventory procedure (LCI) and the Life Cycle Impact Assessment (LCIA). The LCI procedure describes a production system throughout its values chain and the LCI result quantifies all emission flows to the environment as well as all resource consumption flows (all defined as elementary flows). At the LCIA level, by means of linear-weighted aggregations using Characterization Factors (CFs), elementary flows are translated in terms of environmental impacts such as climate change, depletion of resources, acidification, ionizing radiation or human toxicity...

LCIA methods are associated to ready-to-use sets of impact categories (EC-JRC, 2010b). Impact categories of LCIA methods rely on the characterization models of the environmental issues. The environmental relevance and the scientific validity of the characterization models are constantly challenged to update the best practice (Bare and Gloria, 2006; Hauschild et al., 2013; Huijbregts et al., 2016; Jolliet et al., 2018; Rack et al., 2013; Udo de Haes et al., 1999). The use of different LCIA methods may then lead to disparate results (Dreyer et al., 2003; Monteiro and Freire, 2012; Owsianiak et al., 2014; Pizzol et al., 2011). Owsianiak et al. (2014) showed that disagreements in LCIA results are mainly due to differences in the underlying characterization model, in substance coverage, in relative ranking of the reference substance or due to different spatial or time scales. LCA practitioners often choose a LCIA method (or a subset of impact category proposed by a LCIA method) according to (i) existing guidelines bearing the latest update of LCIA methods, (ii) the context and the user needs guided by the goal and scope of the LCA study, (iii) the modelling choice of the method (the intended purpose, the problem or damage-oriented approach, the covered impacts, the regional and temporal validity of the method…) but also (iv) the habits and the expertise of the LCA practitioner (EC-JRC, 2011; ISO, 2006b; Laurent et al., 2014).

From a data analysis point of view, LCIA reduces the complexity of systems described at LCI result level from several hundred variables (high-dimensional dataset of elementary flows, which makes it difficult to fully apprehend the comparison), to a reduced number of criteria for which systems are described by their performance on a few environmental impact categories (low-dimensional dataset, allowing an easier comparison). LCIA can be viewed as a dimensional reduction technique, inherently linked with information losses, but where each of the resulting dimensions has an environmental meaning.

The aim of this work is to help practitioners select the most appropriate LCIA method with regard to the studied LCI results. The selection of impact categories was examined over a large range of products and impact categories by Steinmann et al. (2016). Based on the maximum amount of variance of results from the impact categories, Principal Component Analysis has highlighted an optimal set of impact categories derived from different LCIA methods. In this paper, a Representativeness Index (RI) is proposed to assess how LCI result information can be captured by the LCIA methods and their own impact categories. This RI does not measure the relevance of the environmental model behind the LCIA methods. It rather offers the possibility to obtain an objective appraisal of LCIA methods with additional information on the completeness representation of inventory results they actually perform and can contribute to LCIA result interpretation. This paper is organized as follows: in Section 2.2, the RI is defined and the algorithm developed from a geometric representation of LCA is presented. This approach is illustrated in Section 2.3 on classic LCIA methods for several electricity mix productions from the ecoinvent database(Moreno Ruiz et al., 2013). Finally, representativeness of impact categories are presented for two electricity mixes through a single LCIA method in order to deepen the interpretation of the RIs.

2.2. Material and method

The proximity relationship between a LCI result and impact category vectors can be studied thanks to the geometrical interpretation of LCA methodology. The proximity measurement – also called Representativeness Index (RI) in the following – is defined and adjusted according to the impact category vector as well as to vector sub-spaces generated by sets of impact category vectors (LCIA methods). The implementation is then presented.

2.2.1. Geometrical representation of LCA methodology

2.2.1.1. Life Cycle Inventories result

LCI result is classically defined in LCA as an inventory vector resulting from the computation of the final demand vector, the technology matrix and the intervention matrix (Heijungs and Suh, 2002). This aggregated LCI result consists in the quantification of n elementary flows, resulting from emissions into the environment and resource extractions, over the whole process tree (the involved life cycle steps). This aggregated LCI result belongs to a $\mathbf{G}$ space of n dimensions where n is the number of different elementary flows. The visualization of LCI result in a vector space generated by an elementary flow basis has previously been suggested by Heijungs and Suh (2002) and Le Téno (1999). Therefore any LCI result can be localized in this $\mathbb{R}^n$ vector space either as a simple data point g_i or as a data vector $\mathbf{g}_i$ with n coordinates $g_{x,i}$ $(x \in \{1, 2, \dots, n\})$. The norm of the LCI result vector is directly linked to the reference flow of its functional unit (e.g. the norm of one kilogram of a given product is one thousand times greater than the norm of one gram of the same given product). The direction of the LCI result depends on the relative proportion of the elementary flows. As a simple illustration, Figure 11.a. represents two LCI, $\mathbf{g}_1$ and $\mathbf{g}_2$, described by two elementary flows (i.e. into a 2-dimensional space, here NO_2 and NH_3 gas emissions).

2.2.1.2. Impact categories

The impact categories are the environmental issues used to characterize, assess and compare production systems. For each impact category (e.g. climate change, particulate matter or resource depletion…), a category indicator is defined (e.g. CO_2 equivalent, PM 2.5 equivalent or antimony equivalent). Elementary flows of the LCI result are converted into a corresponding amount of the category indicator by means of CFs. CF values result from the modelling of environmental concerns and, for a given environmental concern, all related CFs form the characterization model of its corresponding impact category. A j characterization model is then a q_j function that associates a $\mathbf{g}_i$ LCI vector to a $h_{j,i}$ one-dimensional impact result expressed as a category indicator:

$$q_j : \begin{cases} G \to H \\ \mathbf{g}_i \to h_{j,i} \end{cases}$$

$$h_{j,i} = q_j(\mathbf{g}_i) = \sum_{x=1}^{n} q_{x,j} \times g_{x,i} \qquad (1)$$

Where $q_{x,j}$ is the CF for x-th elementary flow.

In mathematical terms, the linear-weighted aggregation performed by an impact category corresponds to a linear form that maps a **G** vector space to a scalar. The **G*** dual space is the n-dimensional vector space of all the linear forms $q_j : G \to \mathbb{R}$. Independently of their environmental meaning, all the characterization models determined by their CFs $q_{x,j}$ ($x \in \{1, 2, \dots, n\}$) belong to the dual space. LCI result and characterization models belong to **G** and its **G*** dual space, respectively. According to the Fréchet-Riesz theorem, a linear form q_j of **G*** can be represented by a unique vector within **G**. The characterization model of an impact category can therefore be associated with a vector $\mathbf{q}_j$ of the **G** space using the CFs as coordinates. As a simple illustration, Figure 11.b. shows two impact categories, particulate matter formation ($\mathbf{q}_1$) and acidification ($\mathbf{q}_2$), in the inventory result space. For the sake of simplification, the term "characterization model of impact categories" will from now on be referred to as the "impact category vector". Also, the same notation $\mathbf{q}_j$ will be applied for the impact category vector transferred from **G*** to **G**.

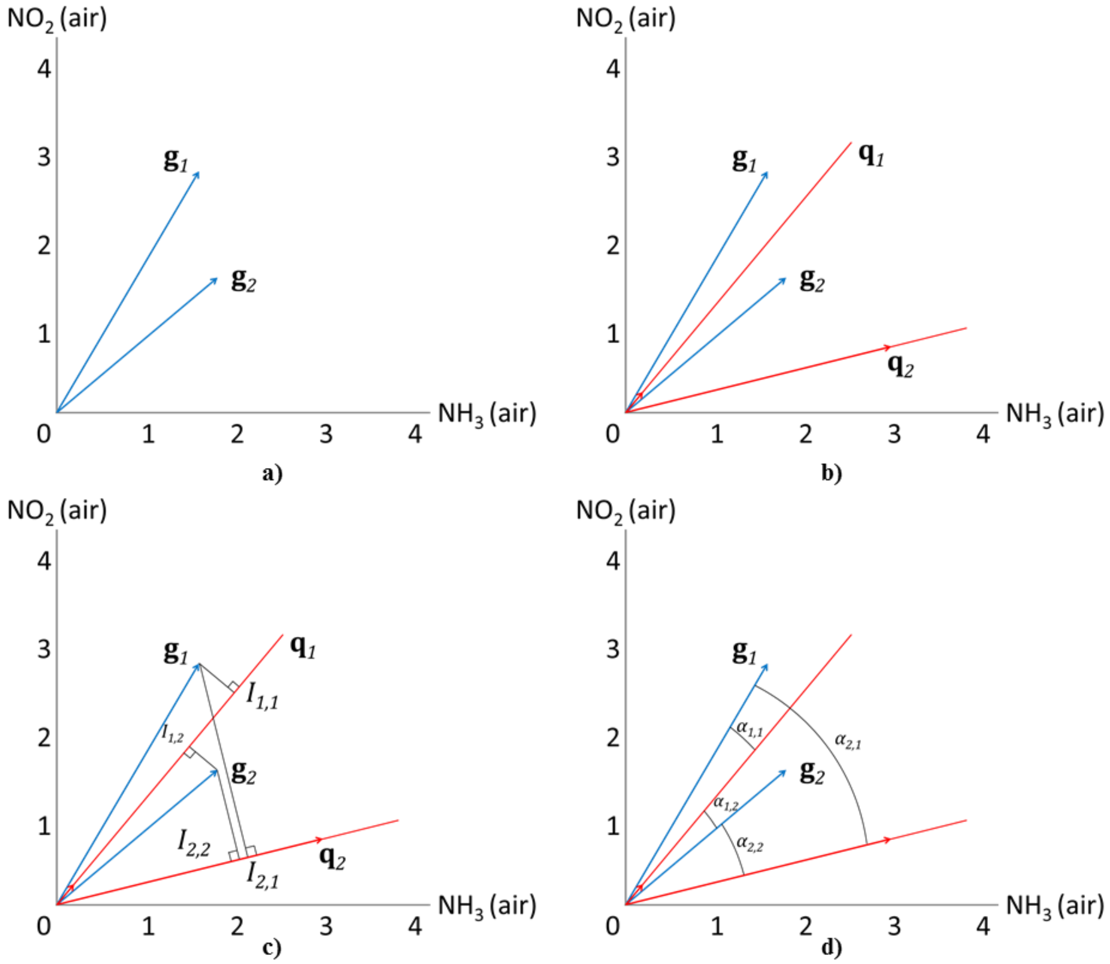


Figure 11. Geometrical representation of LCA: a) Two LCI vectors $\mathbf{g_1}$ and $\mathbf{g_2}$ plotted in a two dimensional inventory space (NO_2 and NH_3 gas emissions in air) ; b) impact category vectors for particulate matter formation ($\mathbf{q_1}$) and acidification ($\mathbf{q_2}$); c) LCA results; d) angular distances between inventories and impact category vectors.

2.2.1.3. Geometric interpretation of Life Cycle Impact Assessment

By representing LCI results and impact category vectors in the same vector space, the LCIA result $q_j(\mathbf{g}_i)$ (or $h_{j,i}$) is then assimilated to the scalar product $\langle \mathbf{q}_j, \mathbf{g}_i \rangle$ between the $\mathbf{g}_i$ LCI vector and the $\mathbf{q}_j$ impact category vector. Figure 11.c. represents the orthogonal projections OI of two $\mathbf{g}_1$ and $\mathbf{g}_2$ LCI result vectors on the two $\mathbf{q}_1$ and $\mathbf{q}_2$ impact category vectors. The coordinates and the norm of $\boldsymbol{OI}_{j,i}$ are easily related to the value $h_{j,i}$ of the impact result (i.e. the scalar product of $\mathbf{q}_j$ with $\mathbf{g}_i$):

$$\boldsymbol{OI}_{j,i} = \frac{\langle \mathbf{q}_j, \mathbf{g}_i \rangle}{\left\|\mathbf{q}_j\right\|^2} . c_j = \frac{h_{j,i}}{\left\|\mathbf{q}_j\right\|^2} . \mathbf{q}_j \qquad (2)$$

$$\|\boldsymbol{OI}_{j,i}\| = \frac{\langle \mathbf{q}_j, \mathbf{g}_i \rangle}{\|\mathbf{q}_j\|} = \frac{h_{j,i}}{\|\mathbf{q}_j\|} \tag{3}$$

Figure 11.c. shows LCIA results visualized through LCI result projections on the impact category axis. Projections of the LCI results on impact category vectors are closer to the $\mathbf{g}_1$ and $\mathbf{g}_2$ LCI result for the particulate matter ($I_{1,1}$ and $I_{1,2}$) than for the acidification category ($I_{2,1}$ and $I_{2,2}$). This implies that, if only one impact category has to be studied as in the example presented in Figure 11, particulate matter would be the most appropriate choice from a data analysis point-of-view to represent the LCI result produced information. Obviously, this does not provide any information regarding the possible environmental drawbacks of the particulate matter concern compared to the acidification concern. If an inventory and its projection are superimposed, the associated impact categories capture all the elementary flow information. On the contrary, a large distance between an inventory and its projection implies that the corresponding impact category poorly reflects the LCI result data.

2.2.2. Definition of a Representativeness Index

The directions of LCI result vectors in the *G* space are driven by the elementary flows and the directions of impact category vectors are driven by the modelled harmfulness of elementary flows for the environmental concerns. By measuring the proximity between a LCI vector and an impact category vector or between a LCI vector and a vector sub-space generated by a LCIA method (a set of LCI vectors), the faithfulness of LCIA results in representing the LCI result can be assessed. It would then be possible to select suitable impact category vectors or a suitable LCIA method according to the studied LCI results. The developed RI is first presented for a LCI result with an impact category vector and secondly with a LCIA method.

2.2.2.1. RI of an impact category

Measuring the distance between multidimensional data sets is common in data analysis techniques (Leskovec et al., 2014). The most common measurement between two vectors is the Euclidean distance. It can be used to measure the proximity between the extremity of $\mathbf{g}_i$ and the extremity of $\mathbf{q}_j$ or the extremity of $\mathbf{g}_i$ and $I_{j,i}$. However, the Euclidean distance is sensitive to the norm of $\|\mathbf{g}_i\|$. Considering two LCI results pointing in the same direction but bearing different norms, the Euclidean distances measured with the same impact category vector would then be different, despite the fact that their elementary flows are similarly represented. To measure the distance between directions, the angular cosine distance hence appears as the most convenient metric to RI.

Defining $\alpha_{j,i}$ as the angle formed by the directions of LCI $\mathbf{g}_i$ and the impact category vector $\mathbf{q}_j$ (see 2-dimensional space example Figure 11.d.), RI is defined as:

$$RI(\mathbf{q}_j,\mathbf{g}_i) = \left|\cos\left(\alpha(\mathbf{q}_j,\mathbf{g}_i)\right)\right| = \left|\frac{\langle \mathbf{q}_j,\mathbf{g}_i\rangle}{\left\|\mathbf{q}_j\right\| \cdot \left\|\mathbf{g}_i\right\|}\right| \tag{4}$$

Because $\mathbf{g}_i$ and $-\mathbf{g}_i$ are identically represented by an impact category, the absolute value of the angular cosine is used. When the RI is close to one, LCIA results carry the major part of the LCI result information (the projection of $\mathbf{g}_i$ on $\mathbf{q}_j$ is close to $\mathbf{g}_i$); conversely, when RI tends towards zero, the LCIA result does not handle the inventory correctly.

2.2.2.2. RI of a LCIA method

Considering $\mathbf{Q}$ as a LCIA method, $\mathbf{Q}$ defines a non-orthogonal multidimensional sub-space generated by its p impact vectors $\mathbf{q}_j$ ($j \in \{1,\dots,p\}$). As previously performed on a single impact category, the projection of a LCI vector can be done on a LCIA method sub-space and the proximity between the LCI and the sub-space can be measured.

In Figure 12, considering a vector space generated by three elementary flows (unit vectors are not presented for reasons of clarity), a 2-dimensional sub-space $\mathbf{Q}$ generated by a LCIA method comprising two impact categories $\mathbf{q}_1$ and $\mathbf{q}_2$ is plotted. The LCIA result of $\mathbf{g}_1$ includes $I_{1,1}$ and $I_{2,1}$, the results from each impact category. The orthogonal projection of $\mathbf{g}_1$ on $\mathbf{Q}$ ($\mathbf{g}_{1,\mathrm{Q}}$) is the part of the inventory which is captured by the LCIA method. The unrepresented part can be measured by the angle $\alpha_{Q,i}$ formed by $\mathbf{g}_i$ and $\mathbf{g}_{i,Q}$, and collected by the RI (eq 5). The RI of the method is an assemblage of the RIs from its different impact categories (see Chapter 3).

$$RI(\mathbf{Q},\mathbf{g}_i) = \left|\cos(\alpha_{\mathrm{Q},i})\right| = \sqrt{1 - \left(\frac{\left\|\mathbf{g}_i - \mathbf{g}_{i,\mathrm{Q}}\right\|}{\left\|\mathbf{g}_i\right\|}\right)^2} \tag{5}$$

If the elements of $\mathbf{Q}$ are independent and orthogonal, $\mathbf{g}_{i,\mathrm{Q}}$ can be considered as the result of the least squares regression $\mathbf{g}_{i,\mathrm{Q}} = \mathbf{Q}\mathbf{y}$ where $\mathbf{y}$ is the projection of $\mathbf{g}_i$ in the $\mathbf{Q}$ subspace. The distance $\mathbf{g}_i\mathbf{g}_{i,\mathrm{Q}} = \left\|\mathbf{g}_i - \mathbf{g}_{i,\mathrm{Q}}\right\|$ can then be easily defined as the residual ($\mathbf{g}_i = \mathbf{Q}\mathbf{y} + \mathbf{g}_i\mathbf{g}_{i,\mathrm{Q}}$). The impact categories of LCIA methods are obviously dependent; many emissions have more than one environmental drawback, thus implying that the characterization factors cover several impact categories. In order to employ the residual of a least squares approach to determine $\mathbf{g}_i\mathbf{g}_{i,\mathrm{Q}}$, the subspace of the $\mathbf{Q}$ LCIA method must be expressed with independent vectors: these are a set of orthogonal vectors $\mathbf{Q}^{\perp}$ which can be obtained through a Gram-Schmidt process.

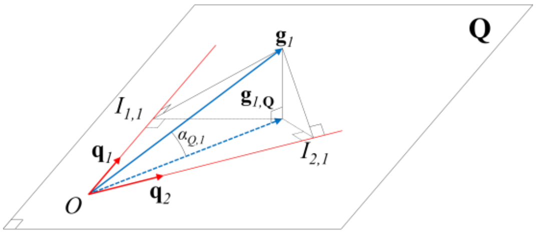


Figure 12. Visualisation of LCIA results and measurement of the cosine distance within a 3-dimensional space

2.2.3. Pretreatment

In LCI results databases, elementary flows are quantified using several units (e.g. kilograms, Becquerel or Joules). In many cases, when a same unit is used, elementary flows present different orders of magnitude (e.g. within ecoinvent, fossil carbon dioxide emissions to the atmosphere are close to 1 kg for most of the LCI results while benzene emissions to surface water are close to 1 µg). A pre-treatment is necessary, if all elementary flows are assured to equally discriminate LCI results within a database and hence if the dependence between measurement units and orders of magnitude and representativeness must be avoided. Classic approaches include min-max normalization, decimal scaling or z-score (most commonly used, optimal for Gaussian distribution). Unfortunately, the first two techniques are sensitive to the presence of outliers while z-score is not appropriate for lognormally distributed data (Qin and Suh, 2016). Preference is given to the scaling of dimensions according to their geometric mean (the mean of the logarithms) because it transforms elementary flows into a common numerical range:

$$\tilde{g}_{x,i} = \frac{g_{x,i}}{\sqrt[m]{\prod_{l=1}^{m} g_{x,l}}}, \forall i \in \{1, \ldots m\}, x \in \{1, \ldots n\} \tag{6}$$

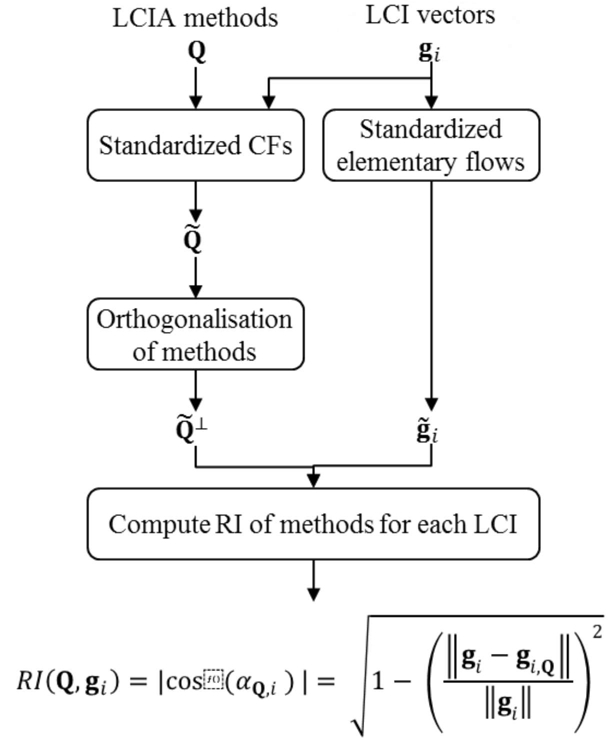
CF units are expressed in kg indicator equivalents per kg of elementary flow; therefore to keep consistent with the units, CFs become:

$$\tilde{q}_{x,j} = q_{x,j} \times \sqrt[m]{\prod_{l=1}^{m} g_{x,l}} \tag{7}$$

The standardization of impact categories transforms them in such way that high standardized CFs correspond to dimensions that are significant for the impact category and for the whole database.

2.2.4. Overview of the approach and implementation

Figure 13 summarizes the full procedure to compute the RI of LCIA methods. Data cleaning is only presented in Figure S 1 of Annex A as it is carried out before the standardization step (data cleaning indeed mainly deals with the nomenclature of elementary flows). Both datasets (LCIA methods and LCI results) are first standardized using the geometric mean of each dimension. The consequences of the LCI result standardization on the directions are illustrated in Figure S 2 of the Annex A. The LCIA method sub-spaces are then orthogonalised through a Gram-Schmidt process. RIs of LCIA methods regarding each LCI result are finally calculated using the results of a least squares regression. To determine the RIs of impact categories, the same procedure is followed except that orthogonalisation is not required.



$$RI(\mathbf{Q},\mathbf{g}_i) = |\cos(\alpha_{\mathbf{Q},i})| = \sqrt{1-\left(\frac{\|\mathbf{g}_i-\mathbf{g}_{i,\mathbf{Q}}\|}{\|\mathbf{g}_i\|}\right)^2}$$

Figure 13. Schematics of the procedure

2.2.5. Material

LCIA methods are ranked according to their RIs over the entire ecoinvent 3.1 database “allocation at the point of substitution” (Wernet et al., 2016). This version of the database was released in 2014. This database comprises 11,276 aggregated LCI result vectors that are described through 1,869 elementary flows (the intervention matrix). The vector space G therefore has 1,869 dimensions.

The LCIA methods are extracted from the SimaPro 8.1.1.16 software to analyse the most recent and operational version. Single-criteria and supersede methods are not considered; only current multi-criteria methods are selected, which represents eighteen classic LCIA methods: ILCD V1.05, CML-IA baseline V3.02, TRACI 2.1 V1.02, BEES+ V4.05, Impact 2002+ V2.12, Ecological Scarcity 2013 V1.01, EPD system 2013 V1.01, EPS 2000 V2.08, EDIP 2003 V1.05 and ReCiPe V1.11 midpoint (mid), endpoint at impact level (end-imp) and aggregated at damage level (end-dam) for egalitarian perspective (E), hierarchist perspective (H) and individual perspective (I) version (Bare, 2011; EC-JRC, 2010a; Frischknecht and Sybille, 2013; Goedkoop et al., 2009; Guinée et al., 2001; Hauschild and Potting, 2005; Jolliet et al., 2003; NIST, 2007; Steen, 1999a, 1999b). The CF nomenclature was transferred from the SimaPro nomenclature to the ecoinvent elementary flows nomenclature with the assistance of the ecoinvent centre that provides us a translation file.

Based on the studied ecoinvent database, electricity production mixes serve as an illustrative example. Four inventories referring to the market production of 1 kWh of high voltage electricity are used. The market version of these LCI results models the aggregated environmental flows of electricity production mixes, transmission networks and electricity losses during transmission. The Chinese and French mixes were chosen because of the prevailing production of hard coal and nuclear power, respectively (see Annex A Figure S 3). The German mix and the area covered by the Northeast Power Coordinating Council (NPCC, North-eastern North America, U.S. only) were analysed because of the diversity of the power supplies that do not individually exceed 34% of the mix.

Implementation was conducted with Python 2.7 on a Jupyter Notebook (formerly IPython Notebook, Perez and Granger, 2007) and using the numerical computation libraries SciPy, Pandas, Matplotlib. The implemented procedure is available upon request from the first author.

2.3. Results and discussion

This section firstly presents the results on the representativeness of LCIA methods for each of the studied LCI results. Secondly, RIs are compared between the different LCI results in order to assess the LCIA method that would be most suitable for comparison. Finally, the RIs of the impact categories within a LCIA method are investigated.

2.3.1. RI analysis of each LCI result

The RI results of the eighteen LCIA methods, analysed using the procedure described in Figure 13, are presented in Figure 14. Along the x-axis, LCIA methods are simply sorted in alphabetical order.

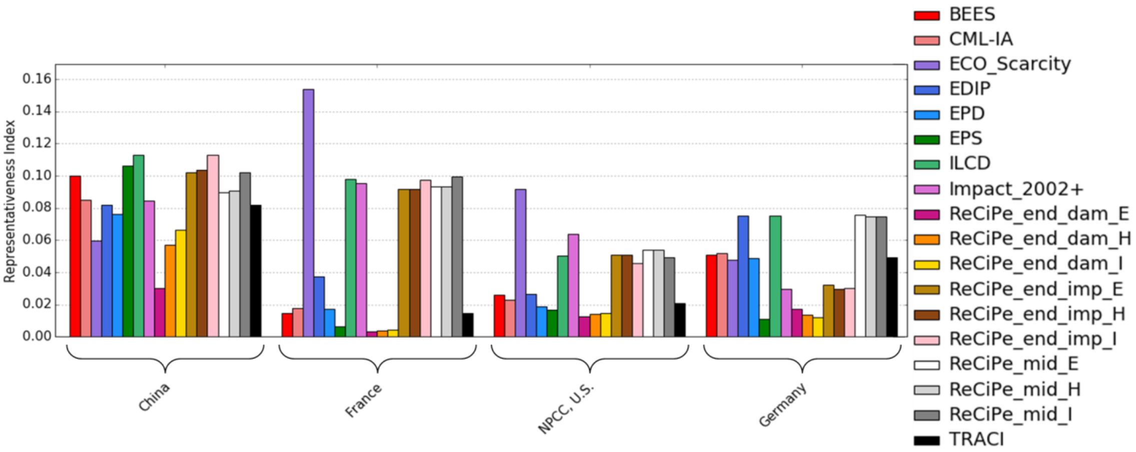


Figure 14. RI of LCIA methods for four electricity mix productions

The Chinese mix production appears to be well represented by several LCIA methods, where the two most suitable are the ILCD and ReCiPe_end_imp_I. For this electricity mix, RIs decrease gradually from 0.11 to 0.03 with ReCiPe_end_dam_E. (see Annex A Figure S 4 for ordered method by decreasing RI values). However, this decrease in RIs is not correlated with the number of impact categories per method: although the 3 ReCiPe_end_dam methods (H, I and E) are each composed of 3 damage indicators and the Ecological Scarcity comprises 18 impact categories, they all get equivalent RIs. This illustrates that the information from the high standardized elementary flows of a LCI result can be well represented by a LCIA method with a small number of impact categories.

Considering the French mix production, Ecological Scarcity outranges all other methods. For the other methods, three main groups can be distinguished. The first group consists of 8 LCIA methods with RIs ranging from 0.09 to 0.10. The second and third groups include 4 LCIA methods with RIs ranging from 0.014 to 0.018 and from 0.003 to 0.006

respectively. The RI for the EPD method stands on its own between the second and third groups.

RIs for the NPCC mix production show a similar trend when compared to the French mix production: Ecological Scarcity also represents this LCI result well and the same first group of LCIA methods is observed around 0.05. However, no group can be distinguished here within the lower RIs showing a gradual decrease for the remaining methods.

Finally, the German mix production shows 4 groups of LCIA methods with EDIP, ILCD and the three ReCiPe Midpoint methods as the most representative LCIA methods with RIs close to 0.075.

This illustrative example demonstrates how RIs present differences for each LCI result. When analysing one specific LCI result, it is possible to determine the most appropriate and representative LCIA method. This study also reveals a set of LCIA methods with equivalent RIs (3 groups for the French mix and 4 groups for the German mix). The methods that constitute a group can be similar in one way or another (similar environmental concerns taken into account within the methods, or similar characterization models, for example). RIs values can be related to the number of impact categories but this has not been observed for all the four LCI results analysed in the illustrative example (see Annex A Figure S 5).

2.3.2. Comparison of RIs of LCIA methods

The purpose of LCA is to be used as a comparison approach; and for a couple of LCI results, both RIs must be investigated (see Figure 15). The most representative LCIA methods for two LCI results get high and similar RIs which localise them close to the first bisector. For example, when comparing the Chinese and the French mix productions (upper left chart), the Ecological Scarcity RI is high for the French mix but distant from the first bisector. This implies that with this LCIA method, the Chinese mix could be underrepresented compared to the French mix, and this could weaken result interpretation. A set of methods (The ReCiPe mid., the ReCiPe end. imp., the ILCD and the Impact 2002+) seems to be a good compromise to compare these two LCI results according to their representativeness. The impact 2002+ might be better for comparing the Chinese and NPCC mixes. The EPD method could be noteworthy for the comparison between the Chinese and German mixes. The Ecological Scarcity method could be relevant for the French and the NPCC representativeness. To compare RIs from more than two of these LCI results is more challenging although the methods that are the most representative of all the LCI results are the ILCD and ReCiPe Midpoint. Results presented in this figure could therefore be decisional support information very easy to understand for the choice of the most representative LCIA method.

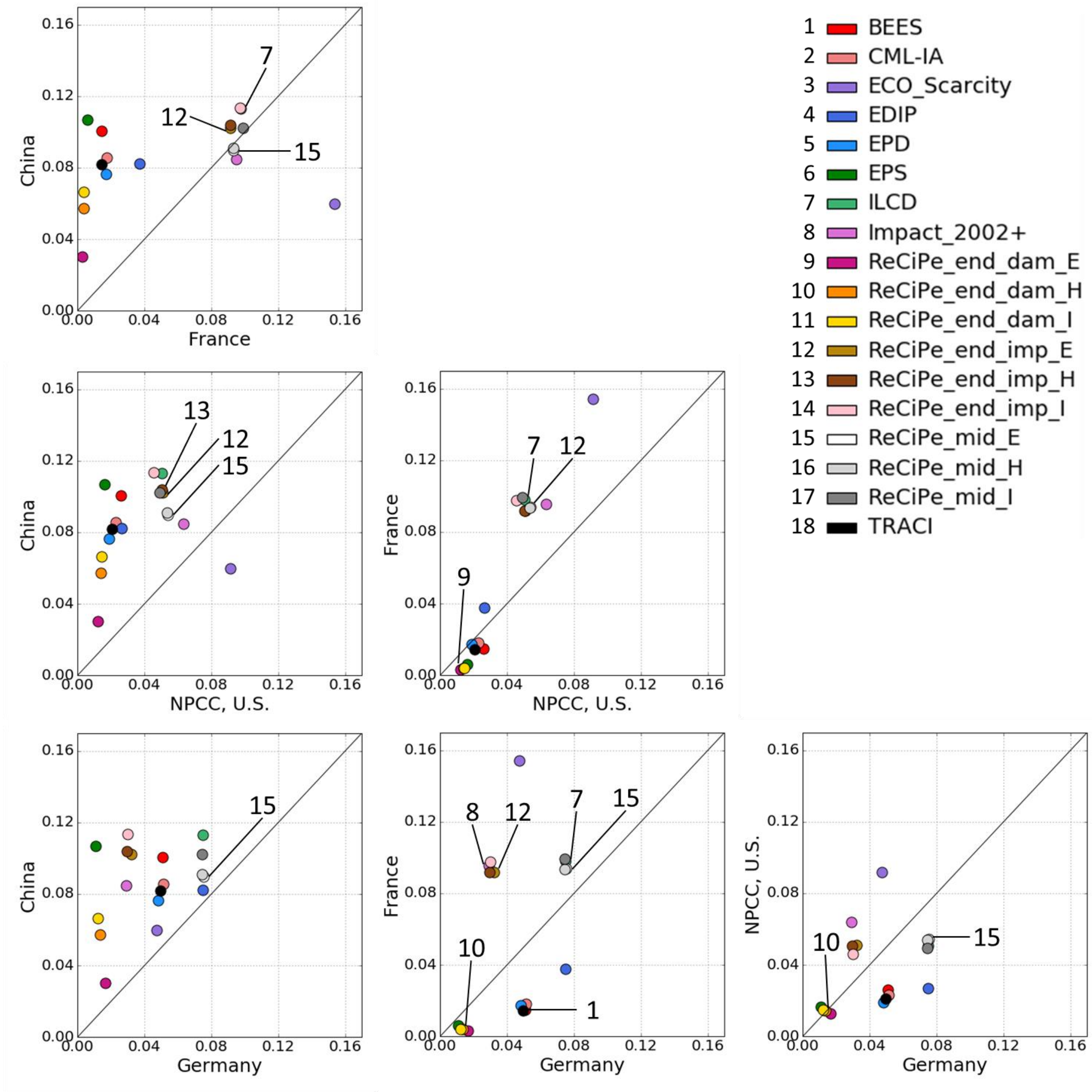


Figure 15. Comparison of LCIA method RIs (numbers indicate the corresponding overlapped points)

2.3.3. Analysing RIs of impact categories

This work focuses on the representativeness of the LCIA method and not on the impact categories to study. However, to fully understand the links between impact category RIs and LCIA method RIs, Figure 16 presents the impact category RIs of the ReCiPe mid. I. method for the Chinese and the French production mixes. This LCIA method appeared as one of the most representative methods for both of them. RIs are here determined for each impact separately. The same information on elementary flows can be represented by different impact categories due to correlations between impact categories.

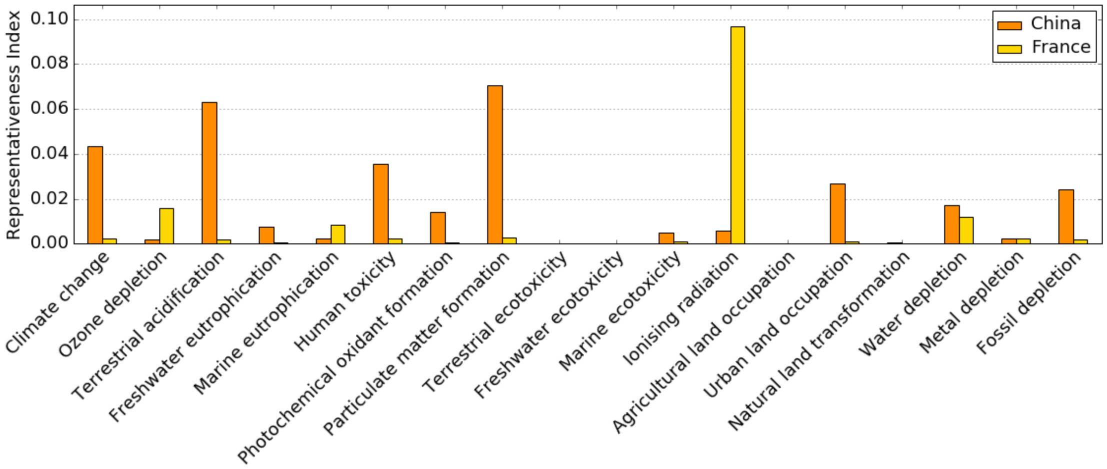


Figure 16. RIs of the impact categories of the ReCiPe mid. I. method for the Chinese and French electricity mix productions

For the Chinese production mix, the first three main impact categories that represent the inventory are particulate matter formation, the terrestrial acidification and climate change. These three environmental concerns are assessed in most of the LCIA methods, which is why this LCI result is quite well represented (Figure 14). The results are quite consistent, given that this production mix is driven by hard coal production.

For the French production mix, the RI of the ionizing radiation category is higher. Within this method, only one impact category represents the main part of the LCI result. As a consequence, the analysis of the environmental impact of this LCI result might not be relevant if methods that do not take this environmental concern into account are used, such as Bees, CML-IA or Traci methods.

The present focus on Chinese and French mixes implies that for certain LCI result such as the Chinese mix, several impact categories are needed to reach an acceptable representativeness of the elementary flows. On the contrary, the French mix is globally mono-criterial with the ionizing radiation category that outranges the representation of this LCI result compared to the other impact categories.

2.4. Conclusions

This work provides a first step in the representation of LCI results by LCIA methods from an algebraic point of view. With the RI measurement, the relevance of LCIA methods used to study the environmental profile of one production system or several production systems within their own database can be compared. Neither the scientific nor the environmental relevance of the LCIA method model is assessed here. The case study shows how LCIA methods can be discriminated on the basis of the information of the studied LCI results that they represent. It reveals that some LCIA methods with a small RI overlooked the main environmental issues of the LCI results. After adapting the implementation and resolving the database nomenclature issues, this methodology could be used by LCA practitioners to compare the adequacy of their own LCI result with the different LCIA methods. Additionally to the practitioner’s knowledge, justifications towards the LCIA method could partly rely on RIs. Results suggest also that the representativeness of impact categories can be variable within a single LCIA method. A LCA study that focuses on a small set of representative impact categories, and not on a complete LCIA method, could lead to further relevant conclusions and interpretations of the environmental results. The RI could then be part of the solution of the impact category selection. Finally, the application of this methodology to specific fields of activity (see Chapter 4) or to compare the global suitability of methods for different LCI results databases, could lead to the establishment of generic guidelines on the use of LCIA methods or impact categories to analyse given LCI results. These guidelines could rely on descriptive statistics of the RIs across different fields of activity.

Chapter 3: A tool to guide the selection of impact categories for LCA studies by using the Representativeness Indexes

Contents of Chapter 3

The previous chapter consisted on the presentation of the RI measurement and its application for LCIA methods selection. This measurement is here used for the selection of impact categories that are worthwhile to focus on. A study case on two electricity mix production LCI results is proposed to present the potential benefits of such measurement for LCA practitioners. The links between the global RIs of LCIA methods and the RIs of their impact categories raised orthogonal issues and an algorithm is then proposed to overcome it. Finally, an interpretation of the standardization procedure leads to study LCI result patterns and defines environmentally critical dimensions.

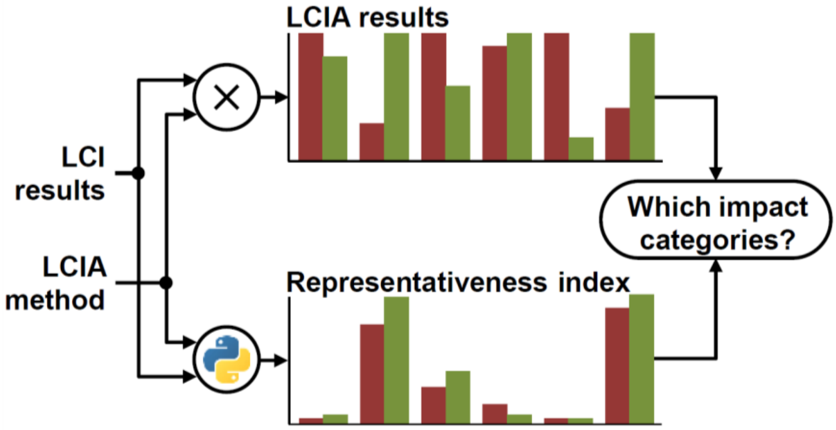


Figure 17. Graphical abstract of Chapter 3

3.1. 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, 2006b), 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 multi-linear 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 products results from the cumulated ecoinvent database (Wernet et al., 2016). Main tendencies of RI results over the cumulated LCI database are then explored. The main representative dimensions that support most of the RI values are then determined. Finally, results from the decorrelation algorithm are analysed over the entire cumulated LCI database.

3.2. Material and method

3.2.1. RI methodology

3.2.1.1. Standardization and definition of an inner product

As proposed by several authors (Esnouf et al., 2018; Heijungs and Suh, 2002; 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 i^{th} product, can be described as a vector $\mathbf{g}_i$ (see Figure 18. a.). However, 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 emphased by Heijungs (2017) about Steinmann et al. (2017) approach; see the section 2.1.2. and Annex B - 1 for details). Defining G_x as the geometric mean of the x^{th} elementary flow, so

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

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

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

Note that we used the absolute value in equation 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 Figure 18.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 part 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). Figure 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 j^{th} impact category for the i^{th} 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:

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

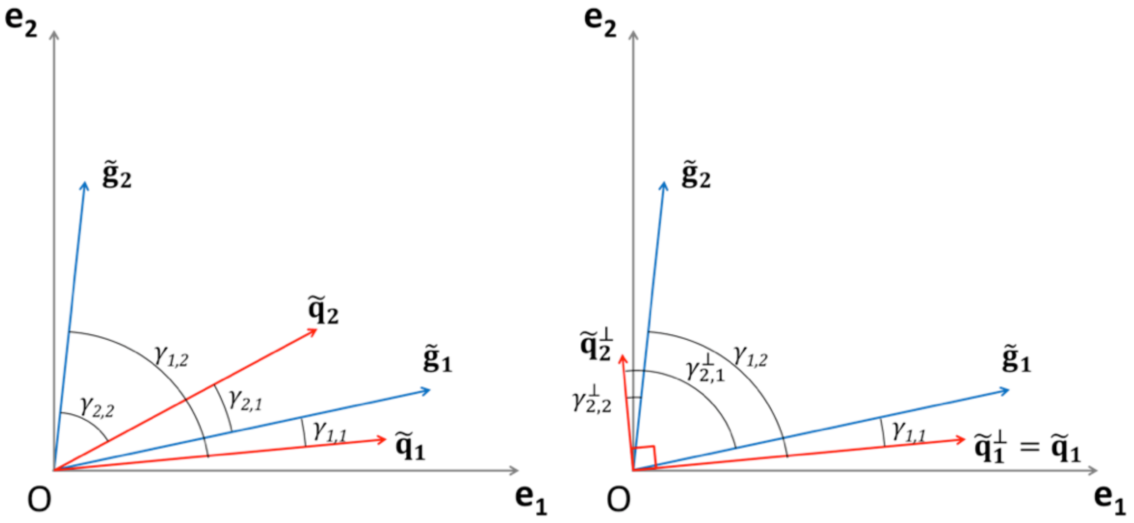
We extend the definition of the inner product of two standardized LCI vectors, say, $\langle \tilde{\mathbf{g}}_1, \tilde{\mathbf{g}}_2 \rangle$ to the inner product of two standardized impact categories, say, $\langle \tilde{\mathbf{q}}_1, \tilde{\mathbf{q}}_2 \rangle$, and to the inner product of a standardized LCI vector and a standardized impact category $\langle \tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i \rangle$ (previously used in equation 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.

3.2.1.2. 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:

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

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.



a) b)

Figure 18. 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).

3.2.1.3. 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:

$$\mathbf{Q} = (\mathbf{q}_1 \quad \cdots \quad \mathbf{q}_p) \qquad (10)$$

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

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

3.2.1.4. 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 Figure 18.b.). Similar to equation 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 equations 9 and 12:

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

and

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

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 Figure

19. 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 Figure 19). 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:

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

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 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 Figure 19).

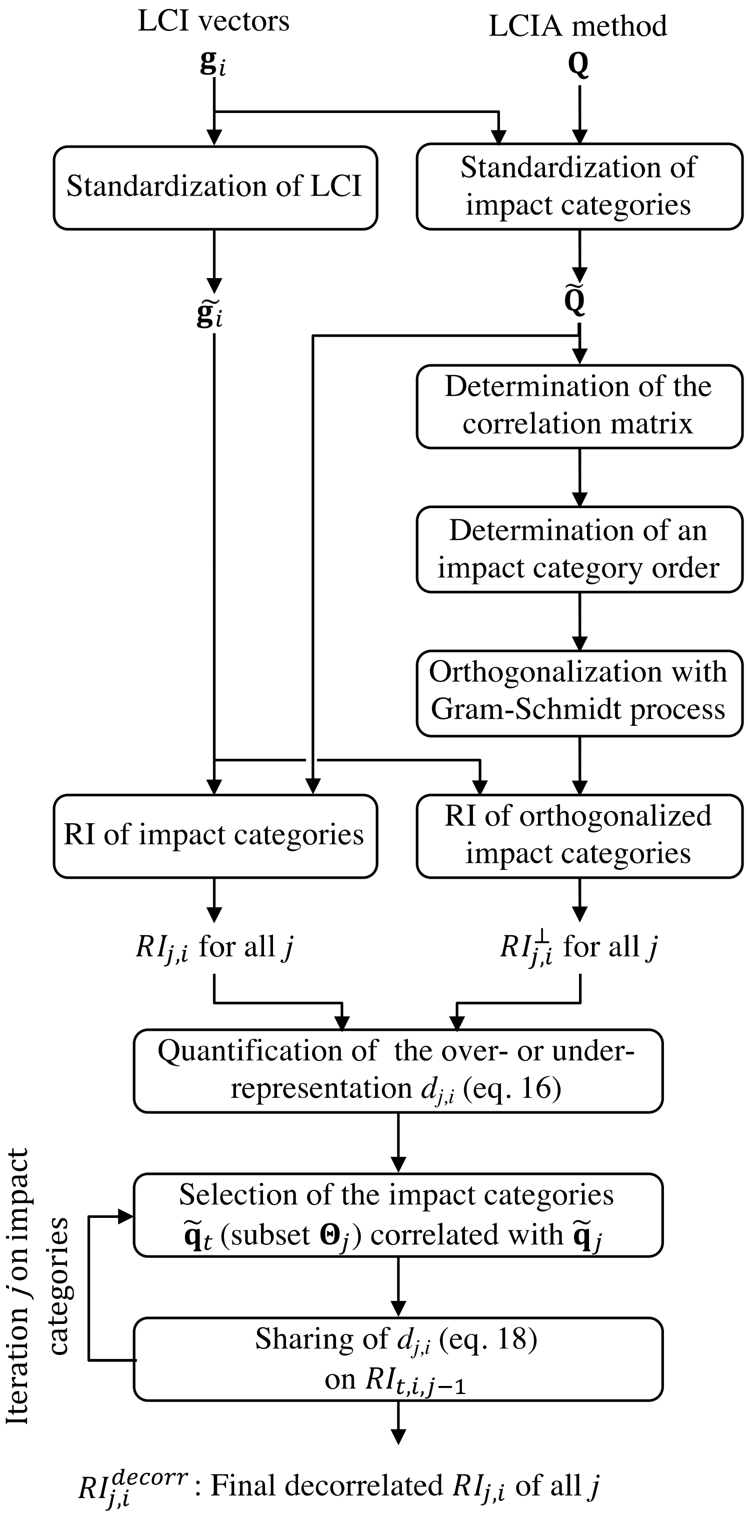


Figure 19. Schematics of the proposed algorithm

3.2.2.5. 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 ($RI_{\mathrm{j,i}}$). Their distance $d_{j,i}$ (as defined in equation 14) 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:

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

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 $\tilde{\mathbf{q}}_j$, $\Theta_j = \{\tilde{\mathbf{q}}_t \middle| t \in \{1, \dots, p\}, r(\tilde{\mathbf{q}}_t, \tilde{\mathbf{q}}_j) \neq 0\}$. $RI_{t,i,j}$ 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 j^{th} 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 equation 9:

$$RI_{t,i,1} = RI_{t,i} \tag{17}$$

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 $d_{j,i}$:

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

At the end of the iteration procedure, all the resulting decorrelated RIs, $RI_{j,i}^{\mathrm{decorr}} = RI_{t,i,p}$, 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.

3.2.3. 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 1,727 elementary flows (the intervention matrix). The elementary flows vector space therefore has 1,727 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 Note-book (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: 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.

3.3. Results and discussion

3.3.1. Illustrative example

3.3.1.1. 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 Figure 20). 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 Annex B - 6). 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 Figure 20, 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 Figure 20) 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.

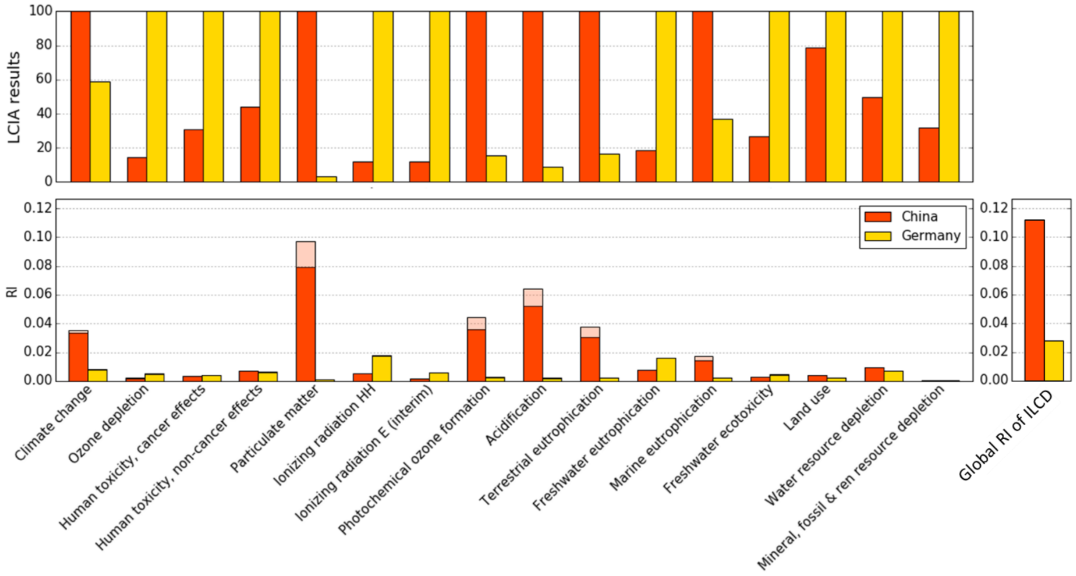


Figure 20. LCIA results (expressed relative to the highest value) and impact category RIs for the LCI results of the Chinese and German electricity mixes from the ILCD method. Bright colours correspond to decorrelated RIs $\boldsymbol{RI_{j,i}^{\mathrm{decorr}}}$ while pastels colours indicate the part removed from the original RIs by the decorrelation procedure, $\boldsymbol{d_{j,i}}$.

3.3.1.2. 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 the Figure 20. Using the $RI_{j,i}$, the equation 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 show the dependences between the impact category vectors, which are removed by the presented algorithm.

Six impact category RIs are particularly affected by decorrelation (see Figure 20). The algorithm lowers the representativness 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.

3.3.2. 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 Figure

21). 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.

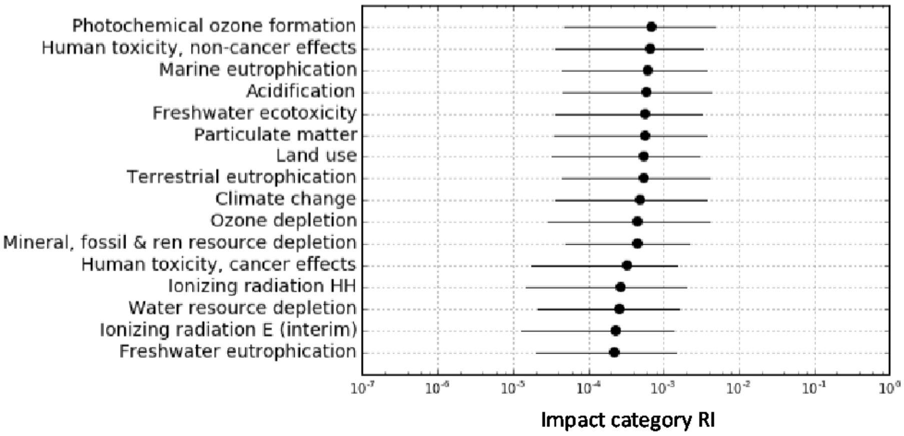


Figure 21. Range of RI values of the ILCD impact categories regarding the LCI results of ecoinvent. Figured are: the median (black dot), the first and third quartile (black segment). Impact categories are classified according to their median.

3.3.3. Contribution analyses of impact category RIs through elementary flow and CF values[1]

Considering a given LCI result and a single impact category, Annex B - 3 illustrates how the impact category RI result relies on the best compromise between elementary flows and CFs. This value is highly driven by one dimension (elementary flow or CF), which is, most of the time, the one with the highest CF of the impact category (see Annex B – 8 and 9). These high standardized CFs are the environmentally critical dimensions of the database for the studied impact categories. According to the resulting LCI result patterns (see Annex B - 2), most of the main elementary flows are probably not involved in the RI value: i.e., they do not correspond to these high standardized CFs. These high CFs point to the dimensions and support most of the RI values. However, only one dimension per category cannot explain all of the RI values and, depending on each LCI result, a combination of dimensions (high elementary flow or high CF) is obviously essential (see Annex B - 3).

---

[1] This section was not published within the paper related to this chapter. In this following section, the term "dimension" refers to a dimension of the **G** vector space were impact category vector have been localized. Then, LCI result vectors and impact category vectors take value on the same dimensions through their standardized elementary flows and their standardized CFs.

For 11 206 ecoinvent LCI results, their representative dimensions, the dimensions which provide 95% of their RI values, were determined (see Annex B - 9). A combination reaching a maximum of 10 dimensions is obtained for land use: a combination of 10 or less dimensions provides 95% of all the RI values (Table 1, column 1) with a global average of 3.17 dimensions (column 4). Considering Climate change, a combination of maximum seven different dimensions is sufficient to obtain 95% of the RI values and its average number of representative dimensions is 3.37. This impact category has a total of 62 non null CFs, although only half of them are present within the representative dimensions of the database: 31 dimensions are present at least in one combination to reach 95% of a single RI. However, most LCI results possess the same representative dimensions, which are obviously strongly related to the higher CFs of the concerned impact category (see Annex B - 9). Considering Resource depletion, almost all of its dimensions are present in at least one RI. Conversely, Toxicities and Ionizing radiations present the highest differences between numbers of non-null CF values and numbers of representative dimensions (see Table 1), which shows that it is almost always the same dimensions that drive the RI value.

Table 1. Descriptive values for the analysis of the main dimensions of RIs

Impact category	maximal number of representative dimensions per LCI	number of different dimensions for 95% of the RIs	number of dimensions with CF ≠ 0	average number of representative dimensions
Climate change	7	31	62	3.37
Ozone depletion	8	14	19	3.10
Human toxicity, cancer effects	6	46	218	2.49
Human toxicity, non-cancer effects	8	64	434	3.36
Particulate matter	7	19	26	4.24
Ionizing radiation HH	4	9	56	2.00
Ionizing radiation E (interim)	5	6	25	1.60
Photochemical ozone formation	8	59	130	4.28
Acidification	8	11	13	4.54
Terrestrial eutrophication	6	10	11	3.15
Freshwater eutrophication	6	9	11	2.18
Marine eutrophication	7	16	25	3.36
Freshwater ecotoxicity	7	94	624	3.37
Land use	10	66	76	4.63
Water resource depletion	3	3	3	1.97
Mineral, fossil & ren resource depletion	8	80	92	3.11

Finally, the RI values per number of dimensions per combination were investigated. Results for the Climate change category are presented in Figure 22 (similar figures are presented in Annex B - 4 for the other impact categories). As previously observed in Table 1 (column 1), 7 dimensions is the maximal amount of representative dimensions per combination.

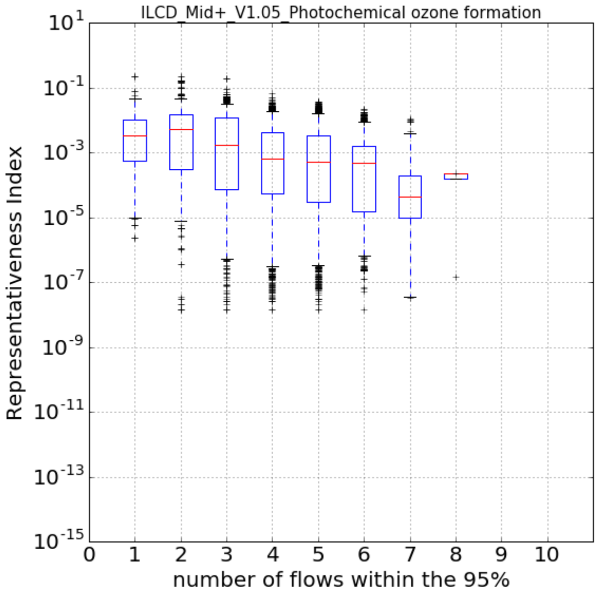


Figure 22. Boxplot of RI distributions according to the amount of dimensions per combination to represent 95% of the information.

A slight decrease in RI values is observed when the number of required dimensions increases for this impact category (this is also observed for almost all impact categories). Most of the LCI results that only require one dimension to reach 95% of their RI present a high RI value. These LCI results have a very high intensity for the same dimension that drives the impact category vector. When more dimensions are required within 95% of the value, the RI values decrease. Using Annex B - 9, the same representative dimensions that are generally found to be involved (due to high CFs) although LCI results have a lower intensity for these dimensions.

These analyses reveal that only a few dimensions out of the entire cumulated LCI database provide values for a large part of the RIs. They are the most critical and representative dimensions through which the modelled human activities in ecoinvent impact most of the time on the environmental issues of the ILCD. The high RIs reveal the LCI results that have high standardized elementary flow values on these critical dimensions. The lower RIs therefore provide insights on the elementary flow values of the LCI results on these critical dimensions.

3.3.4. Decorrelation of impact category RIs within a LCIA method

3.3.4.1. 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.

Table 2. Correlation matrix of impact categories of the ILCD method, on the basis of 11206 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

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

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.

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}). The nitrogen oxide dimensions dominate the CFs on subset B. This observation is critical for the Photochemical ozone formation category (see Annex B - 8). Excepting for the high chromium VI and Zinc CFs that relate both human toxicities and freshwater ecotoxicity impact categories, the dimensions on which the correlations of the subset A are based do not correspond to the dimensions associated with major CFs for these impact categories. This can explain the low correlation indexes within this subset.

3.3.4.2. Consequences of decorrelation over the cumulated LCI database

Orthogonalized impact category RI values are obtained by applying the algorithm to all 11206 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 $\frac{RI^{\text{decorr}} - RI}{RI}$ are analysed for each impact category; see Figure 23. Distributions of the ratio are based on the original RI values and the orthogonalized RI values of the impact categories (see equations 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.

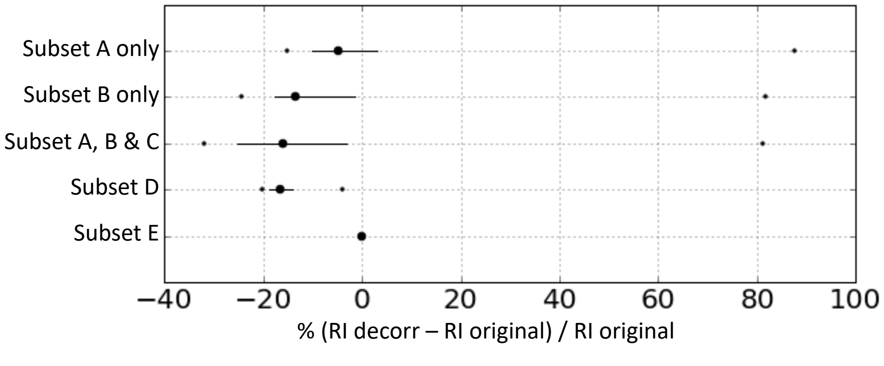


Figure 23. Analyses of the different redistribution of RI values. Ordinate refers to the belonging of the impact categories. Shown are: the median (large dot), the first quartile (left end of line), the third quartile (right end of line), and the 5% and 95% percentiles (small dots).

Results imply that the major part of the redistribution slightly decreases the RI values from $RI_{j,i}$ to $RI_{j,i}^{\text{decorr}}$ (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 a 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 Figure 23.

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 Annex B - 5).

The increase of RI values for $RI_{j,i}^{\mathrm{decorr}}$ is triggered by the high $RI_{j,i}^{\perp}$ which is observed for several subsets. A LCI result with an 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 Figure 18.b). When LCI results have a high value on this second elementary flow, their $RI_{j,i}^{\perp}$ tend to increase compared to $RI_{j,i}$. Most of the LCI results characterized by higher $RI_{j,i}^{\perp}$ originate from agricultural production.

Dimensions such as NMVOC (non-methane volatile organic compounds), ammonia, nitrate or ethene seem to represent the main secondary dimensions that trigger the increase of RIs for the A, B and C subsets when the CFs from the orthogonalized impact categories are analysed. Most of the LCI results characterised by RI increases originate from agricultural production. This is mainly related to ammonia and nitrate dimensions. The redistribution of extra information from the secondary dimension should provide the impact categories of the subset with an increase that finally allows their $RI_{j,i}^{\mathrm{decorr}}$ to comply with the RI of the LCIA method.

3.4. 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.

Chapter 4: Representativeness of impact categories in LCA according to fields of activity

Contents of Chapter 4

In this chapter, we explore if the RI methodology puts forward distinct LCIA methods and environmental issues while analysing relatively homogeneous datasets based on subtypes of products and activities. Analysis of RIs of all impact categories from classic LCIA methods shows interesting trends that could lead to provide guidelines for LCA practitioners regarding the 14 studied fields of activity.
To avoid redundancy in the thesis between chapters, this chapter is not fully formatted as a publishable article. Reminders on context and method will be added so that the article can be read independently.

4.1. Introduction

Life Cycle Assessment (LCA) is an interesting approach to assess and compare all the potential environmental impacts of human activities (ISO, 2006a, 2006b). The elementary flows linked to the different productions of products or services constitute Life Cycle Inventories (LCI) result. LCI results are then translated in term of environmental impact through the Life Cycle Impact Assessment (LCIA). However, a large number of LCIA methods has been developed over the past decades and offer a wide choice of environmental indicators (Hauschild et al., 2013). Each of them has its own specificities, characterization models, spatial and time scales (Owsianiak et al., 2014) which can puzzle LCA practitioners when a LCIA method and its impact categories have to be chosen during the goal and scope definition phase of their studies.

LCI results databases as ecoinvent 3.1 (Wernet et al., 2016) gather a wide diversity of human activity models as for example from wheat grain production to high-speed train transport. Several studies already proposed to test statistical procedures, as selection or redundancy of indicators, by sampling LCI results depending on their field of activity. Huijbregts et al. (2006) classified around 1218 LCI results segregated through four fields of activity from the ecoinvent database V. 1.2: energy production, material production, transport and waste treatment. Environmental impact scores were then analysed with linear regression to explore correlation with a fossil energy based indicator. Fields of activity proposed by the ecoinvent database V.2 were analysed by Pascual-González et al. (2016) to uncover the relationships between environmental indicators. Steinmann et al. (2016) carried out a principal component analysis on 976 LCIA results of “cradle to gate” LCI results segregated in seven product types. Distinct distributions on principal component scores were obtained per product category. Two product categories (oil and electricity) from ecoinvent, that gather a total of 231 LCIA results, were studied by Pascual-González et al. (2015) with a combination of multi-linear regression and mixed-integer linear programming to predict impact category results. Results showed that working with homogeneous set of LCI results leads to different sets of LCIA metrics and different number of LCIA metrics needed to predict the other ones.

However, these works focus on the LCIA results and do not handle the LCI result vector space. The Representativeness Index (RI) presented in Chapter 2 assesses the appropriateness of a LCIA method and each of its impact categories for any given LCI result. For a studied LCI result, the RI measurement relies on the contextualization of the LCI result (see Chapter 3) and the impact categories and (at the elementary flow and the characterization factor level) in regard of its database from which the studied LCI result is modelled. The angular proximity between a LCI result and the impact categories is the measure of relevance of the impact category (see Chapter 2 and 3).

The previous chapters provide RI results for specific case studies using four and two LCI results. This chapter focuses on the RI results by segregating LCI results based on their field of activity. With a systematic approach, we explore if the RI methodology puts forward distinct environmental issues per field of activity. Before the modeling of a LCI result, these results can provide to the LCA practitioner a first estimation of the main representative impact categories associated to the involved processes. It will be on the main dimensions of these categories that the modeling effort will have to be done. Then once the LCI result is modelled and its main representative impact categories obtained, it can bring elements of discussion by comparing the representative impact categories of the studied LCI results and the representative impact categories of the field of activity.

This paper is organized as follows: in Section 4.2, the developed measurement from the RI methodology is briefly reminded and the LCI results grouping procedure per field of activity is presented. In Section 4.3, the results of the global RI of the ILCD method are presented, followed by the analysis of the RI distributions of its 16 impact categories. Finally, RI results between fields of activity are compared with enlarging the analysis to 18 LCIA methods which gather 232 impact categories.

4.2. Material and method

4.2.1. RI methodology

The present work takes place within the same formalization of the LCA framework as described in Chapter 2. For each LCI result and regarding the frame of reference of the LCI results database, the RI measurement assesses the intensity of each of its elementary flows and compares this intensity to the critical dimensions of a set of impact categories. This assessment allows revealing the representative impact categories (or the representative LCIA methods) regarding a LCI result. In this chapter, we study the same version of the ecoinvent database (Wernet et al., 2016) as in the previous chapters.

Firstly, global RIs of the ILCD methods (EC-JRC, 2011) are determined for the LCI results of different fields of activity. RIs are then measured for its impact categories regarding each LCI result. Secondly, the study is enlarged to other multi-criteria methods: CML-IA baseline V3.02, TRACI 2.1 V1.02, BEES+ V4.05, Impact 2002+ V2.12, Ecological Scarcity 2013 V1.01, EPD system 2013 V1.01, EPS 2000 V2.08, EDIP 2003 V1.05 and ReCiPe V1.11 midpoint (mid), endpoint at impact level (end-imp) and aggregated at damage level (end-dam) for egalitarian perspective (E), hierarchist perspective (H) and individual perspective (I) version. (Bare, 2011; Frischknecht and Sybille, 2013; Goedkoop et al., 2009; Guinée et al., 2001; Hauschild and Potting, 2005; Jolliet et al., 2003; NIST, 2007; Steen, 1999a, 1999b)

4.2.2. Fields of activity study

The modelled activities are divided into 14 fields of activity using the International Standard Industrial Classification of All Economic Activities (ISIC) (United Nation, 2008). This classification proposes different level of grouping: section, division, group and class. For example, the activity of wheat grain production is referred to Section A 0111. It belongs to the Section A 'Agriculture, forestry and fishing', division 01 'Crop and animal production, hunting and related service activities', group 011 'Growing of non-perennial crops', and class 0111 'Growing of cereals (except rice), leguminous crops and oil seeds'.

The present study analyses the RI measurement regarding 9,622 LCI results of the ecoinvent database with a referenced ISIC number. Here, the section level of the classification was used (see Table 3). A splitting with the division code was applied when activities gathered by a section were considered too diversified (see Section C and D) and when the generated subgroups were big enough to determine valuable descriptive statistics. Details of the division level belonging to each field of activity are provided in Annex C – 1.

Table 3. Number of inventories per fields of ISIC activity

Field of activity	Number of LCI results
Section A, Agriculture and forestry	632
Section B, Mining and quarrying	280
Section C, Processed Biobased product	482
Section C, Chemicals and Plastics	1494
Section C, Other non-metallic mineral products	285
Section C, Metals and metal products	564
Section C, Electronic and electronical equipment	355
Section C, Machinery and transport equipment	355
Section D, Electricity power generation	2788
Section D, Manufacture of gas	90
Section D, Steam and air conditioning supply	407
Section E, Sewerage and Waste treatment	1150
Section F, Construction	561
Section H, Transport land	179
total	9622

Subdivisions of Section C "Manufacturing" were needed due to the large range of products covered. These subdivisions were based on the ISIC division level and led to six consistent sets of LCI results (regarding the fields of activity) with enough LCI results each. Section D was split in three to separate the energy carriers (electricity and heat) of the natural gas manufacturing and supply division. The subdivision of Section H led to three subgroups where air and water transports were put aside because of being constituted of only ten LCI results each. Sections not taken into account due to low numbers of LCI (which limit the calculation of descriptive statistics) represent a total of 176 LCI results: manufacture of furniture, air and water transports, telecommunications, real estate activities, architectural and engineering activities, office support activities.

Descriptive statistics are determined on the RI distributions of each field of activity regarding the ILCD method and its different impact categories. Fields of activity are analysed through common non-parametric descriptors as median (range of the median is assessed by its order of magnitudes and its width) and inter-quartiles. This allows comparing the representativeness between fields and between impact categories.

Considering medians as a good indicator of the RI distribution over LCIA method and impact category, basic correlation analyses are finally performed between median values of several fields of activity. The median values of other multi-criteria LCIA methods, that represent a total of 232 impact categories, are finally studied (see details in Annex C - 2). Impact categories related to the same environmental issue are grouped. For example, all impact categories assessing metal, fossil, abiotic, mineral depletion or energy resources but from different LCIA methods are put together within the environmental issue "Resources and energy use". In line with the main categories proposed in the ILCD documentation (EC-JRC, 2011), 12 groups of environmental issue are then created (see Table 4). The goal is to uncover similitude and difference on the RI results of environmental issues from different LCIA methods.

Table 4. Number of impact categories per environmental issues

Environmental issue	number of categories
Land occupation/transformation	21
Climate change	17
Resources and energy use	27
Eutrophisation	20
Acidification	15
Ozone depletion	14
Photochemical oxidant formation	11
Particulate matter formation	12
Ecotoxicity	47
Human toxicity	28
Ionising radiation	14
Water depletion	6
total	232

4.3. Results and discussion

4.3.1. Study of the ILCD

4.3.1.1. Global RIs of the ILCD per field of activity

Global RIs of LCI results regarding the ILCD method are first analysed. The RI distributions per field of activity and over the database are presented in Figure 24 (data are provided in Annex C – 3). A ranking is applied from the median of RI values.

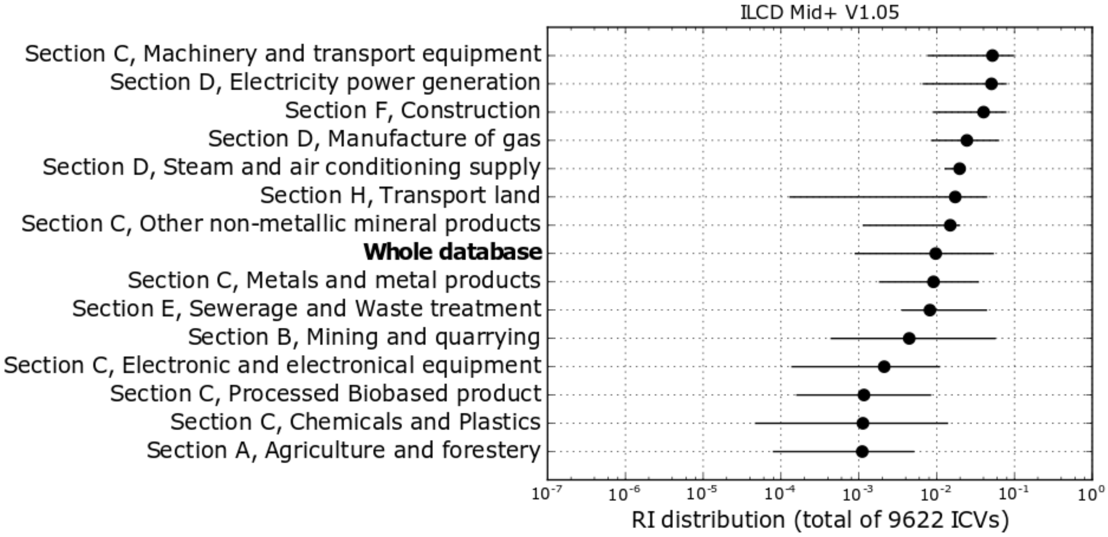


Figure 24. Global RI distributions for fields of activity and the whole database (black dots are the medians, first and third quartiles are represented by the bars. Fields of activity are classified according to their median)

RI distributions show clear distinction and uncover the differentiations of the fields of activity from the database. The medians range from 10^{-1} to 10^{-3} and with considering the larger of the inter-quartiles (from 7 to 3.35 × 10^{2}), an evaluation of the relative appropriateness of the ILCD method between fields of activity can be possible. Gathering all the studied LCI results, the database ranges in the middle of the ranking as it would have been expected. The impact categories of the ILCD represent well the Machinery and transport equipment (MATE) and, at the opposite, the LCI results of the Agriculture and Forestry (AF) products seem not to be very intensive on the representative dimensions of those impact categories. The inter-quartiles show a relatively high variability between fields. It can reveal the high or low heterogeneity of the LCI results pattern within a field. This value is discussed after when analysing impact category RIs.

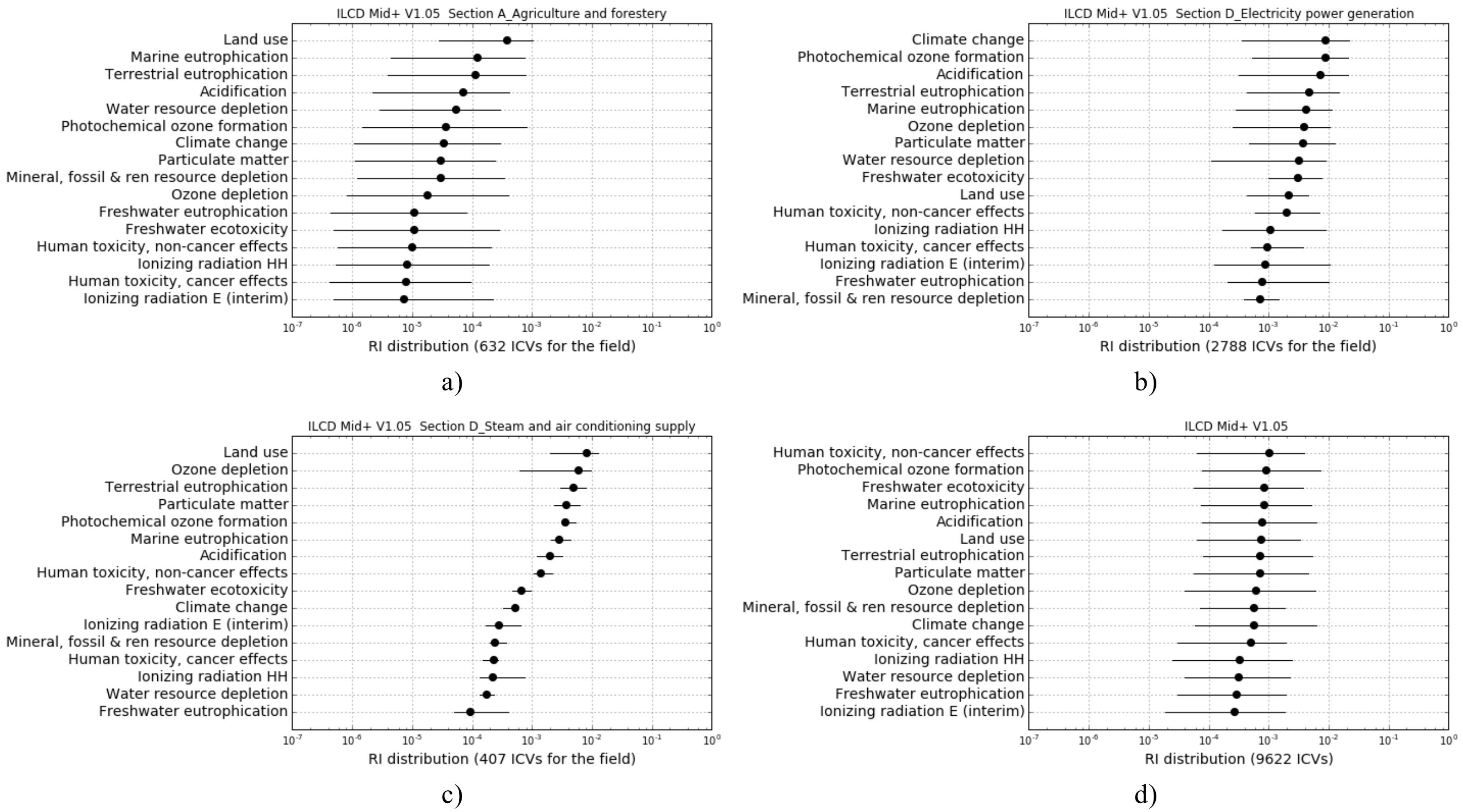
As an illustrative example, let us consider an electricity production from anaerobic digester feed with dedicated agricultural productions (the biomass is produced for energetic purpose). This system takes place mainly in the agricultural sector. If it is put in front of an electricity mix, two activity sectors are involved in the comparison. The ranges of RIs highly differ between both sectors, if the electricity one is well represented, agricultural activities are often poorly represented by the ILCD (see Figure 24). Potential advantages of the anaerobic digestion system should be interpreted cautiously because of the potential misrepresentation of this sector: conclusions should consider relevant impact categories for the agricultural sector (see below) in priority.

4.3.1.2. Distribution of RIs of impact categories per field of activity

Figure 25 presents results of the 16 impact categories for three fields of activity and the whole database: the Agriculture and Forestry (AF), the Electricity Power Generation (EPG) and the Steam and Air Conditioning Supply (SACS). These three fields of activity were chosen because of dissimilar results distributions observed on their global RIs (Figure 24). RIs of impact categories allow uncovering the interesting ones that support the global RIs of the ILCD. Descriptive statistics and figures related to all the other fields of activity are provided in Annex C - 4.

Median values range from 10^{-3} to 10^{-5} for AF. These values are globally higher for the EPG and the SACS fields: ranging from 10^{-2} to 10^{-3} and from 10^{-2} to 10^{-4} respectively. The database gets average values from 10^{-3} to 10^{-4}. As already observed on global RI distributions, studying the ranges of the median values shows clear distinctions between these fields of activity. LCI results related to EPG and SACS are globally better represented by these impact categories than AF. These LCI results are more intensive on dimensions that are also targeted by the impact categories.

The ratio between the minimal and the maximal median values are not similar between fields of activity (also see data in Annex C - 4). This ratio is very low for EPG (maximal median being 12 times greater than the minimal), the AF obtain a lager ratio (48 times) which is even greater for SACS (88 times). A high ratio shows that a clear distinction between high and low representative impact categories could be made. Some impact categories are more representative of the intensive elementary flows of the concerned LCI results than others impact categories. This ratio is finally not very contrasted (3.7 times) when analysing the whole database: all the impact categories are relevant for at least some LCI results.



a) b)

c) d)

Figure 25. RI distributions for three fields of activity and the whole database (black dots are the medians, first and third quartiles are represented by the bars. Impact categories are classified according to their median)

Regarding the inter-quartiles, their distributions are quite variable between fields of activity but are similar within each field of activity. SACS has very narrow distributions (maximum of inter-quartiles: 6.8) while AF has very large ones for all impact categories (maximum of inter-quartiles: 564). The variability of inter-quartiles observed on the global RIs of the LCIA method (Figure 24) was similar of these results. A high variability obtained for AF can be interpreted by the fact that the intensities of these LCI results on the critical dimensions are more variable than for SACS. It reveals a high or low heterogeneity on the LCI results patterns within each field of activity. When the inter-quartiles are large, it might be interesting to study sub-divisions of field separately, assuming that inter-variabilities between sub-parts are larger than intra-variabilities of them. Indeed, the overlapping inter-quartiles can be an issue for the selection of representative impact categories per field and RIs per LCI result might be more relevant to study than studying RI distributions.

Based on the median values, impact category ranking reveal interesting results. Focusing on the first impact categories, this ranking reveals the environmental issues that are most of the time considered as relevant by expert when studying LCI results belonging to the respective fields of activity. The land use, the marine and terrestrial eutrophication and the acidification indicators are put forward for the AF. This gives the key concerns for the electricity from anaerobic digestion system to focus on, in addition to climate change, photochemical ozone formation and acidification, which are targeted by the EPG. For this field, the very low rank of resource depletion can be surprising but it is due to the fact that this ILCD indicator gives higher importance on indium (a critical mineral raw material) and other mineral than on fossil fuels. Within the SACS field, a high number of heat productions from wood resources are actually present. This can explain why the land use ranks first for this field. The intensities of LCI results on CFCs used for cooling productions might also be responsible for the ozone depletion rank. Terrestrial eutrophication and particulate matter are put forward due to emissions related to steam and heat production (nitrogen oxides, particulates, sulfur dioxide). The number of interesting impact categories per field of activity seems to depend on the ratio between the maximal and the minimal median value and the overlapping of inter-quartiles between impact category RIs. As the ratio of extreme medians is small for the whole database while inter-quartiles are very large, the impact category ranking (Figure 25.d.) may not be meaningful and point out that all categories are needed.

Knowing the field of activity of a LCI result, medians and inter-quartiles of RIs determined from the other studied LCIA method might lead to support the selection and provide guidelines toward the 18 LCIA methods and the main impact categories

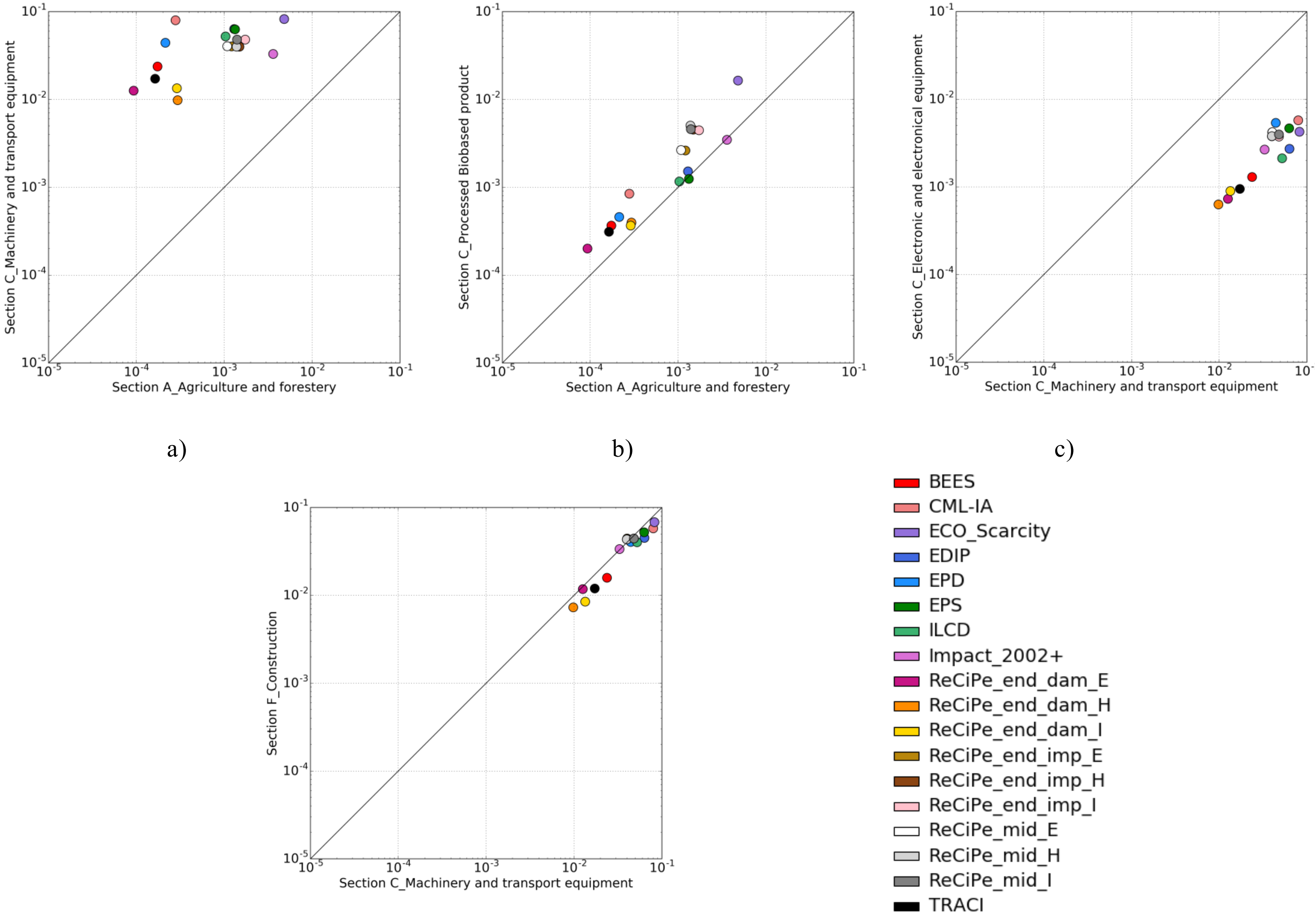
4.3.2. Exploring RI distributions within other LCIA methods

4.3.2.1. Comparison of RIs of LCIA methods

We extended the global RI analyses to other LCIA methods. Comparison of median values from the distributions of global RIs per field of activity regarding 18 LCIA methods are presented in Figure 26. Biplots reveal the relative appropriateness of each LCIA method regarding the different fields of activity and allow visualizing correlations. Through the different environmental indicators measured within each LCIA method, relevance of LCIA methods differs for a given field of activity.

The Ecological Scarcity method (ECO_Scarcity) is ranked as the best LCIA method to use for most of the fields. It is mainly due to the high number of impact categories that is measured by this LCIA method. By aggregating information through 3 indicators, the ReCiPe damage methods are the last representative LCIA methods.

Figure 26.a. shows a sparse cloud of points. The LCIA methods represent with very different manners the information from the MATE and AF fields. As already seen with the ILCD method, the MATE gets globally higher RIs than the AF. The dispersion indicates that LCIA methods target different environmental issues that are more or less representative of the MATE or the AF. On the contrary, other comparisons obtain better correlations: Processed Biobased product – AF (Figure 26.b.); Electronic and electrical equipment – MATE (Figure 26.c.); Construction – MATE (Figure 26.d.). Correlations of global RI results on these fields reveal possible similitude on LCI results patterns from different fields (similitude inter field) and links within their respective values chain.



a)

b)

c)

d)

Figure 26. Comparison of the medians of LCIA method RIs

4.3.2.2. Comparison of RIs of environmental issues modelled within LCIA methods

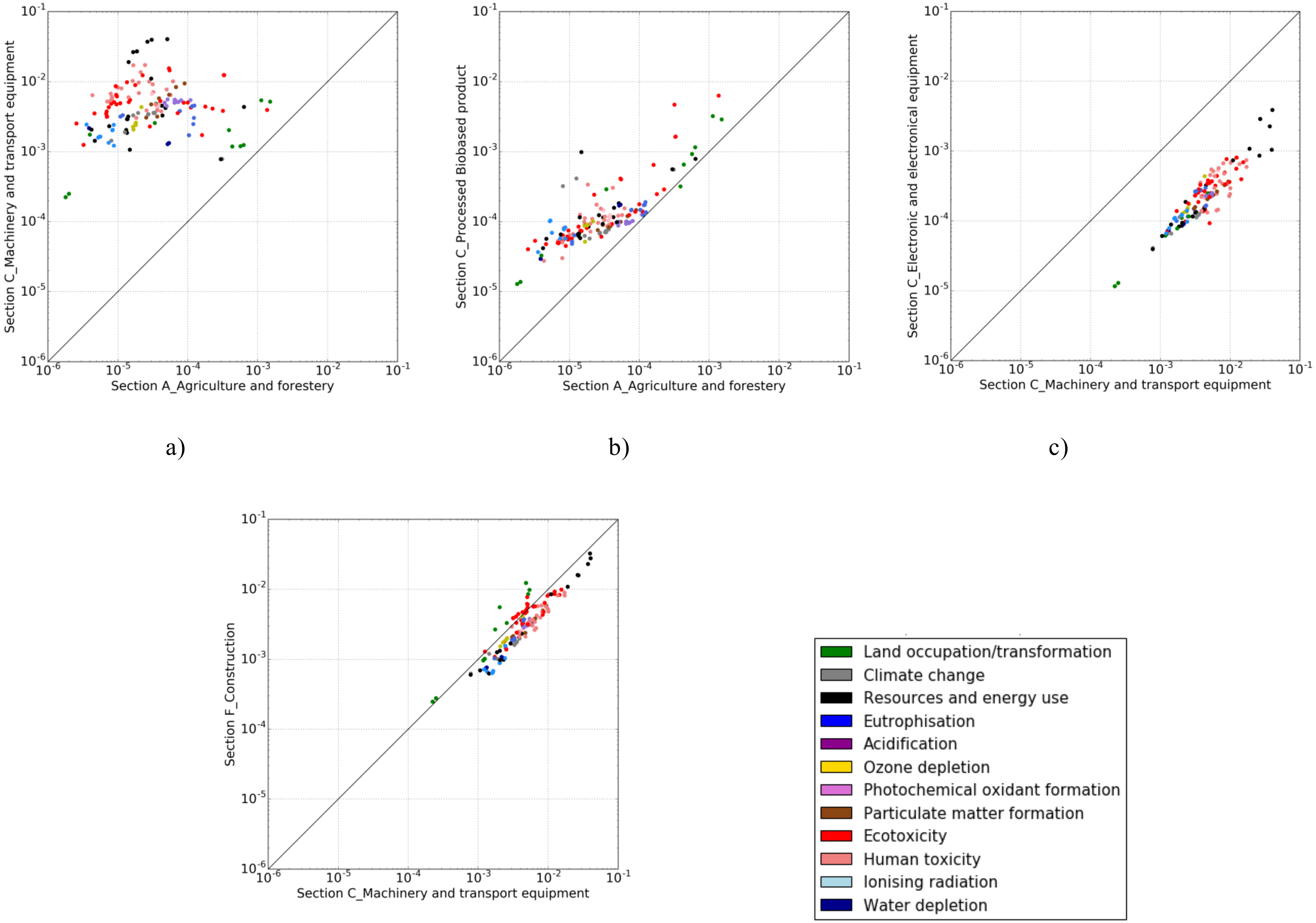
As previously carried out with LCIA methods, relationships between impacts categories regarding different fields of activity are investigated here with correlation analysis on median values of RIs, (see Figure 27). First of all and without considering the environmental issue groups, the correlations of impact categories between fields of activity (low for MATE – AF, Figure 27.a. and high for construction – MATE, Figure 27.d.) are similar to the correlations of LCIA methods. This demonstrates that LCI results patterns from related fields of activity tend to be similar. On the contrary, two fields that are very distinct lead to a dispersed cloud of points. The localizations itself of the clouds of points are also the same as observed for LCIA methods (high RIs for MATE and low RIs for AF), but impact category RIs get smaller values than global RIs of LCIA method. Those observations are direct consequences of the links between the value of the global RIs of LCIA method and impact category RIs (see Chapter 3).

Regarding the environmental issue groups, the acidification, the particulate matter, the ozone depletion, the photochemical ozone formation, the climate change and the ionizing radiation groups show very similar behaviors regarding the distributions of their representation of fields of activity. Medians of these groups are very close. It reveals the potential strong correlations of impact categories that model similar environmental issues from different LCIA methods (Steinmann et al., 2017).

The eutrophication group is segregated in two parts (see blue dots in Figure 27.a. and Figure 27.b.). This division is mainly due to the grouping of marine and terrestrial eutrophication (nitrogen as limiting factor for the ecosystem) with freshwater (phosphate as limiting factor) within the same environmental issue group.

The human toxicity group, the eco-toxicity, the land use and the resources energy use groups show much more dispersed median values. The characterization models behind the impact categories grouped by these environmental issues are very different. As a consequence, the standardized impact categories have different environmentally critical dimensions: their vectors point to different dimensions. For example, the critical dimensions of resource and energy use impact categories are very distinct: indium, copper, nickel, chromium, cadmium, crude oil and natural gas. They show a wide dispersion (black dots in Figure 27.c. and Figure 27.d.), seemingly segregated into two groups for the resource and energy use (mineral and fuels), regarding the representation within each field of activity.

Finally, being grouped by environmental issues, the impact categories show similar ranking as observed in section 3.1.2. regarding each field of activity. Land use and eutrophication groups stand out for AF; and climate change, resource and energy use and photochemical ozone formation groups are put forward for EPG.



a)

b)

c)

d)

Figure 27. Comparison of the medians of impact category RIs

4.4. Conclusion

This paper presents an exploration of the representativeness of LCI results grouped by fields of activity regarding LCIA methods and impact categories. Segregation of LCIA methods and impact categories based on RIs of fields of activity can be possible. We show that, for group of LCI results, some indicators are more relevant to study due to a better representation of the LCI results patterns within the group. Land use, eutrophications and acidification are the best representative impact categories for Agriculture and Forestry products while climate change, photochemical ozone formation and acidification are relevant for Electricity Power Generation processes. Similitude of representativeness of impact categories from different LCIA methods was also observed as in other papers.

However, a limitation of this analysis is due to the relatively high inter-quartiles that are sometimes obtained and thus, the localization of impact categories might not only be resumed by the median value. The global distributions are also interesting while medians and inter-quartiles avoid overlapping distribution within a field of activity. More homogeneous groups might be sometimes more relevant to obtain stronger conclusions.

Another limitation is the redundancy among products within the ecoinvent database. Indeed, within a field of activity, some LCI results from different market or area are very similar. The electricity power generation sector is one of the main sectors affected by this issue. The high number of LCIs that model electricity production mix probably heavily pulls the standardization of the database and the impact category in function of their LCI results patterns. RI distributions might be affected by the over-representation of several LCI results. Fields of activity with very distinct LCI results patterns from the main ones (as Agriculture and Forestry) might endure it by obtaining relatively low RIs. Steinmann et al. (2016) carried out a more drastic LCI result selection before any pretreatment by using only global market product and by discarding LCIs with high pattern similarity.

This work can finally lead to carry out screening of the representativeness of all the impact categories provided by the different LCIA methods regarding the LCI result being studied by a LCA practitioner. Selection of representative impact categories from different LCIA methods and related to different environmental issues could provide relevant composite LCIA method per field of activities.

Chapter 5: Life Cycle Assessment of a biofuel production from cellulosic macro-algae: key aspects for the environmental concerns

Contents of Chapter 5

This chapter applies the RI methodology on the LCA of the production of biofuel from cellulosic macro-algae. First, an inventory of the system developed within the Green AlgOhol project (ANR-14-CE05-0043) is presented and a contribution analysis is carried out with the ILCD method. Then, RIs of the whole system and sub-part of the values chain are studied for the ILCD method. Finally, a RIs screening of classic LCIA methods and their impact categories is performed.
This chapter is not fully formatted as a publishable article to avoid repetitions and will be improved to be read independently.

5.1. Introduction

Providing the world in truly sustainable energy is one of the major concerns that our society has to face during the decades to come. Switching from fossil fuel to biofuel is considered as a promising potential alternative. Among feedstock, new biomasses like algae receive increasing attention as a potential renewable source for biorefinery to produce materials, chemicals or energy (Pandey et al., 2014). All algae have a potential high biomass yield but compared to microalgae, macro-algae can potentially be cultivated in offshore cultivation systems or in simple open raceway systems, and due to their structure, the biomass concentration is made easier by just being harvested (Collet et al., 2015, 2011). While micro-algae have metabolic storage pathways based on lipids, macro-algae are natural producers of starch and unlignified cellulose (Hughes et al., 2012).

New alternatives to conventional energy carrier have to be an improvement from an environmental perspective. Several environmental analysis with Life Cycle Assessment (LCA) were carried out for biofuel productions from macro-algae such as biodiesel (Aresta et al., 2005), methane through an anaerobic digestion process (Cappelli et al., 2015; Langlois et al., 2012; Pilicka et al., 2011; Seghetta et al., 2017) or ethanol through a fermentation process (Aitken et al., 2014; Alvarado-Morales et al., 2013; Brockmann et al., 2015). These studies show the potential of this kind of biomasses for energetic purpose but point out the need of an efficient design of the system face to inputs of the cultivation step (fertilizer, electricity consumption…).

Brown and red seaweeds are already widely used as food and feedstock for biorefinery processes (mainly for agar, carrageenan, and alginates extraction, Bixler and Porse, 2011). However green macro-algae represent a minor part of the actual algae production. Species like *Chaetomorpha* sp. are an interesting biofuel feedstock with the ease of production and high similar cellulose content to that of land-based biomass (Schultz-Jensen et al., 2013).

To tackle the potential of this kind of biofuel production system, this study assesses the environmental performance of a hypothetical system of ethanol production from onshore cultivated green seaweed (*Chaetomorpha* sp.) and its use in a passenger car. All the values chain is considered for this prospective LCA study to uncover the main contributing production steps of the Life Cycle Inventory result (LCI) on environmental indicators. The Representativeness Index (RI) presented in the previous chapter is then used on this LCI result to test the representativeness of the selected LCIA method (in the goal and scope definition phase of the LCA study) and its respective impact categories. Moreover, the representativeness of these environmental indicators is determined on sub-systems of the LCI result. Finally, a screening over other LCIA methods is performed to explore RI results on other environmental indicators.

5.2. System definition and inventory

5.2.1. Goal and scope, and functional unit

The goal of the analysis is the evaluation of the potential environmental impacts caused by bioethanol production from cellulosic macro-algae (*Cheatomorpha* sp.) and its combustion in a passenger car. In a cradle-to-grave perspective, environmental performance is assessed using the standardized LCA methodology. All the steps of the values chain are included: from the algal cultivation to the final use to power a passenger car. This LCI result is assessed to determine the main contributors to the environmental impact of the system. The functional unit of the system is to drive 100 km in a passenger car (medium size). The LCA software Simapro 8.1 has been used for the modeling. The ecoinvent database V.3.1 "allocation at the point of substitution" was used for background processes (Wernet et al., 2016). The characterization of environmental impacts is based on the LCIA method ILCD 2011. Recommended by the European Union (EC-JRC, 2011), the selected LCIA method assesses the environmental impacts at a midpoint level. Due to inconsistencies between the water impact assessment method and ecoinvent v.3.1 database, this impact has been removed from the assessment method.

5.2.2. Life cycle inventory

Figure 28 shows the main steps of the system. System starts from the algal cultivation in open raceways: this step needs a supply of water from the sea and uses up fertilizers. After the harvesting, algae are conveyed to the ethanol production plant. This second main step is composed by pre-treatments and enzymatic hydrolysis of the biomass, and an alcoholic fermentation. Post-treatments (distillation and purification) are then carried out to provide ethanol inline with distribution and use constraint. System ends with the final use to power a passenger car.

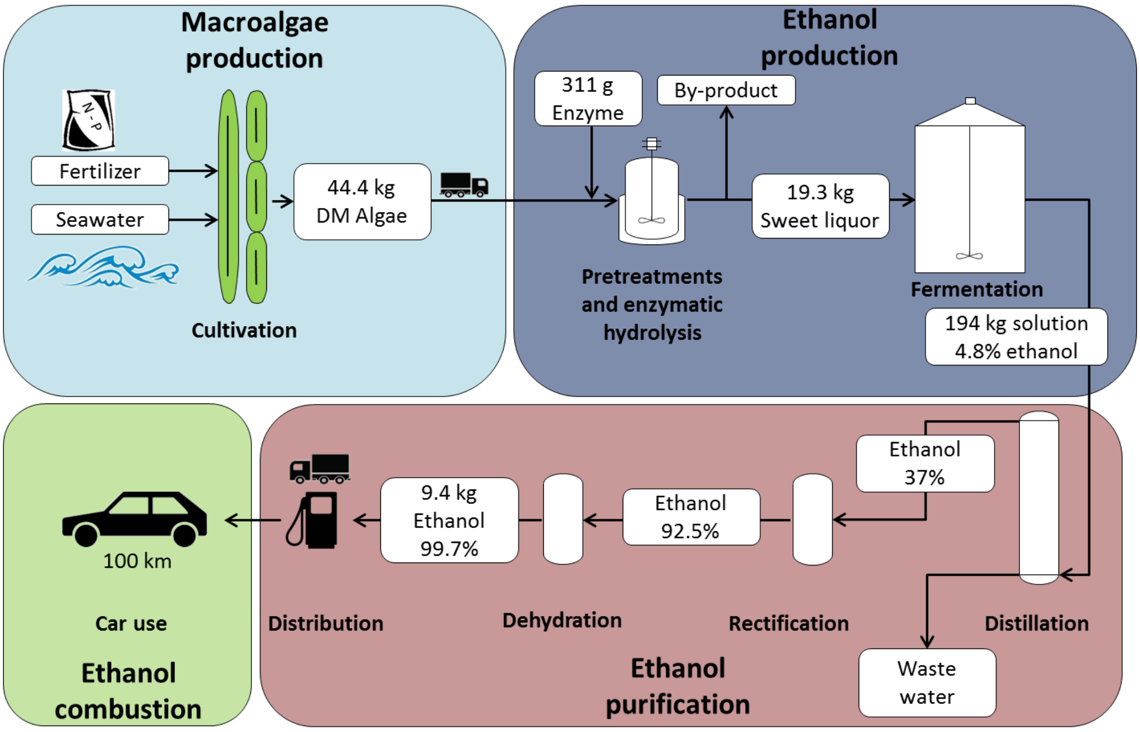


Figure 28. Schematic representation of the values chain

5.2.2.1. Macro-algae production

Production of *Chaetomorpha* is modelled at industrial scale. Due to missing industrial scale facilities for this algae production, this LCI is based on literature data, laboratory scale data and expert knowledge of the system provided by the French Centre for the Study and Use of Algae (Centre d'étude et de valorisation des algues, CEVA). The modelled system produces 11,200 kg of dry matter (DM) of algae per year for a total raceway surface of 9,500 m^2. The production needs 20,500 m^2 of seawater per year and 10,900 kWh of electricity. The French medium voltage electricity mix, mainly based on nuclear energy, is used to power the entire LCI.

Based on laboratory scale data, the growth rate of *Chaetomorpha* is estimated to be 10 g DM /m^2/day with an initial density of 0.5 kg DM/m^2. The dry weight of the grown algae is assumed to be 20%. Algae cultivation is carried out in open raceways where water is mixed by a paddle wheel. Four raceways are considered in this cultivation system. They are all excavated and lined with an EPDM liner of 1.14mm. A large raceway (5,000m^2) is dedicated to the growth period of algae. Every week 350 kg of DM of algae are transferred from the large raceway to a small raceway (three open raceways of 1,500 m^2 each) for a batch of starvation. Two weeks of starvation is needed to stress algae to increase their carbohydrate content (estimation to up to 50% of DM). A cultivation season of 28 weeks is assumed but there are only 23 weeks where a full production is considered: the first 5 weeks are needed to get a minimal quantity of algae to start starvation procedures. Only nitrogen and phosphate are added to seawater during the growth period: ammonium sulfate and phosphate (ecoinvent market processes). Additional details on the infrastructure and industrial amenities can be found in Brockmann et al. (2015).

5.2.2.2. Ethanol production

After the harvest, algae are transported over 60 km by lorry to the ethanol production site. The pre-treatment and the enzymatic hydrolysis of biomass are achieved to make the carbohydrates accessible during the bacterial fermentation step. The pre-treatment and the enzymatic hydrolysis are modelled using the ASPEN software to define infrastructure, industrial amenities, electricity and heat (confidential data, French Petroleum and New Energies Sources Institute, IFP Energies Nouvelles). The enzymatic production is modelled from the ASPEN model proposed at an industrial scale level by NREL (Davis et al., 2013; Humbird et al., 2011). Cellulase is produced through an aerobic fermentation process by *Trichderma reesei*. Glucose needed as input is provided by hydrolyzation of maize starch (Dunn et al., 2012) and nitrogen is provided from corn steep liquor (Mu et al., 2010). After the enzymatic hydrolysis of the algal biomass, a solid-liquid separation step is operated. To obtain a full overview of the whole system with an ecodesign perspective and a complete mass balance, neither allocation nor substitution was taken into account. It remains obvious that co-product management rules will have to be used for comparison to conventional fuel.

Ethanol is obtained through an anaerobic fermentation process of the sweet solution obtain after the solid-liquid separation. The ethanol production is based on the model proposed by NREL. 63% of the carbon of the sweet solution is considered to be transformed into ethanol by *Zymomona mobilis*.

5.2.2.3. Ethanol purification

Distillation, rectification and dehydration of the fermented solution are based on the NREL model. Distillation allows reaching a concentration of 37% of ethanol; rectification increase the titration to 92.5% and then the dehydration makes the titration reaching a suitable value of 99.7% for combustion in an engine. Distribution to service stations is based on a process inventoried in ecoinvent database that takes into account freight by lorry and train.

5.2.2.4. Ethanol combustion

The model of the combustion of ethanol in a passenger car is based on the ecoinvent process 'transport, passenger car, medium size, petrol, EURO 5' for Europe. Fuel consumption is changed for ethanol consumption based on their low heating value: 42.5 MJ/kg for petrol and 28.1 MJ/kg for ethanol (Jungbluth and Chudacoff, 2007): ethanol consumption is then 9.4 kg over 100km. Emissions strictly linked to petrol evaporation (PAH, benzene, toluene, ethene, propene…) and heavy metal emissions per kilogram of petrol used are removed of the inventory. Carbon dioxide, carbon monoxide and methane emissions are considered as biogenic. Other flows (road use, car maintenance, and tire and brake emissions) are not modified considering that the fuel type would not modify them.

5.2.3. Applying the RI methodology

RIs of the ILCD method and its corresponding impact categories are determined for the modelled LCI. The script provided on the online deposit was used (Chapter 3).This analysis tests the representativeness of the selected environmental issues during the goal and scope of the LCA study. Further investigations are conducted on RIs of subsystems of the LCI. Aggregated LCI result of the following four subsystems are obtained from SimaPro: macro-algae production and production, purification and combustion of ethanol. Representativeness of the ILCD method and its impact category are determined for those four aggregated LCI results.

Finally, a screening of the global RIs of other classic LCIA methods and the RIs of their respective impact categories is carried out to check if other indicators tackle a better representation of the LCI result and its subsystems than the ILCD impact categories.

5.3. Results and discussion

5.3.1. Contribution analysis

The results of the contribution analysis are shown in Figure 29. Onshore production and transport of the harvested algae (macro-algae production) contribute for more than 40% to the overall environmental burden for all impact categories, except resource depletion. This LCI step has its major contributions on land use and ionizing radiations categories. The electricity needed to move water and the production of the raceways (excavation and linen use) are the steps that are involved in most this contribution (see Annex D - 1).

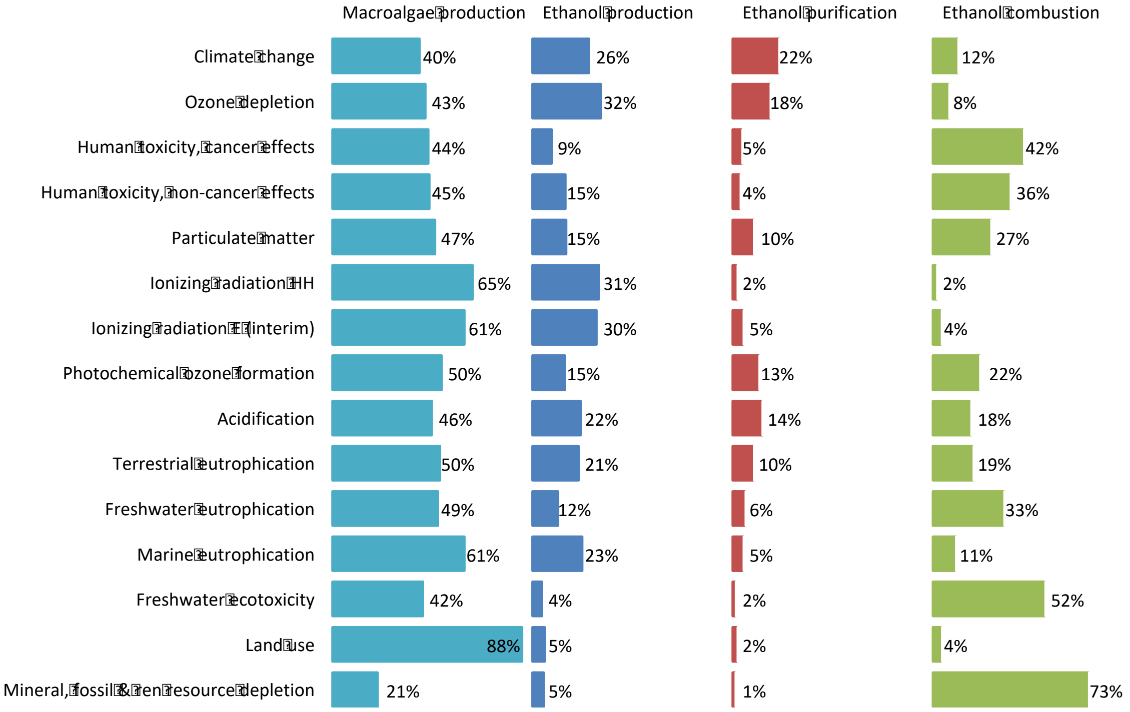


Figure 29. Process contribution analysis

Ethanol production impacts exceed 20% for seven impacts, being the second largest contributor for each. The most contributive step for ethanol production is the pre-treatment and enzymatic hydrolysis step. The heat provided by steam production from natural gas is the environmental hotspot for this process on climate change and ozone depletion. Cooling of the solution is the hotspot on the ionizing radiations. An interesting result is the contribution of starch from conventional maize which is use for cellulase production: human toxicity (non-cancer effects), terrestrial and marine eutrophication are effected to up to 10% by this agricultural step.

Ethanol purification obtains its major contribution on climate change and ozone depletion with around 20% of the environmental burden. Like for pre-treatments, heat production is the process that triggers this result.

Ethanol combustion is the main contributor to resource depletion often the second contributors (for six impacts). Car production is the final step that obtained non-negligible contributions on most of categories. Resource depletion is dominated by indium, tantalum, cadmium and nickel use while chromium VI, copper and zinc emissions drive human toxicities and ecotoxicity results. Being set as biogenic carbon, the carbon dioxide emitted by ethanol combustion does obviously not appear in climate change result.

The major optimization that could be obtained would be on the cultivation step. Increasing yield growth of *Chaetomorpha* and limiting water movements and transfers are the main parameters that would decrease the environmental burden of this step.

5.3.2. RI results

5.3.2.1. RIs of the ILCD

For the entire LCI result, the global RI of the ILCD is 7.75 x 10^{-5}. This value is quite low regarding the distributions obtained in Chapter 4. The environmentally critical dimensions of this LCIA method do not target the highest standardized elementary flow of the LCI result.

Figure 30 presents RI results of the non decorrelated impact categories of the ILCD. As for the global RI of the LCIA method, the impact category RIs are relatively low. The RI methodology reveals that most of the elementary flows on which this LCI result is intense are not on dimensions targeted by the impact categories of the ILCD. The ionizing radiation HH, the land use and the resource depletion categories are the impact categories that are put forward. The first standardized elementary flows of the LCI result are captured by those three impact categories. The environmental burden on those impact categories is due to the electricity that powers the system and the land used by raceways (Annex D - 1). Because the algae production step is the one that most use those processes, its optimization seems to be the highest priority in order to decrease the environmental burden of this scenario.

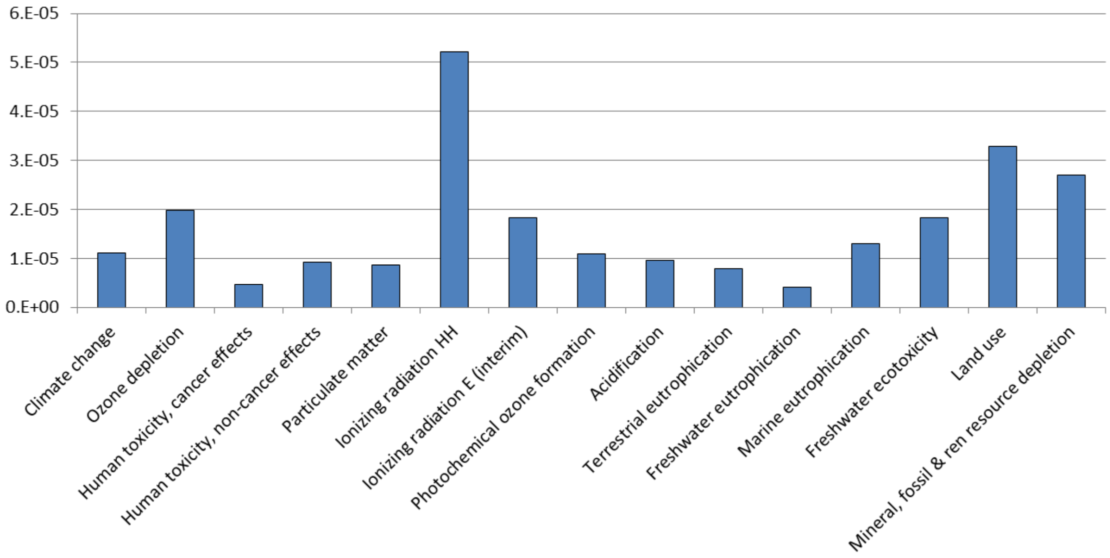


Figure 30. RI results of the entire LCI result

5.3.2.2. RIs of the ILCD impact category regarding the four LCI result subsystems

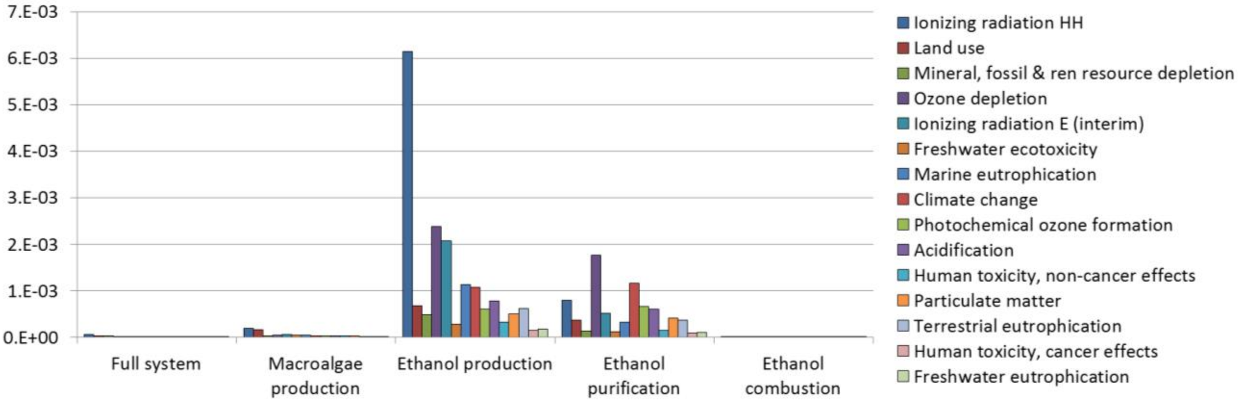
The global RIs of the ILCD method are presented in Table 5 for four subsystems of the LCI result. The first three subsystems, macro-algae production and ethanol production and purification, obtain higher RIs than the entire LCI result. Ethanol production has the highest RI that range close to the median of the RIs of the database (Chapter 4). By extracting subsystems, the LCI results obtain totally different elementary flow patterns: their elementary flow intensities are different from the original LCI result. If a global system can be poorly represented by an assessment method, subparts, considered separately, can be well grasped. Ethanol combustion remains misrepresented by ILCD with a RI of the same order of magnitude than the entire one.

Table 5. RI values of the ILCD method for each subsystem of the biofuel production from macro-algae system.

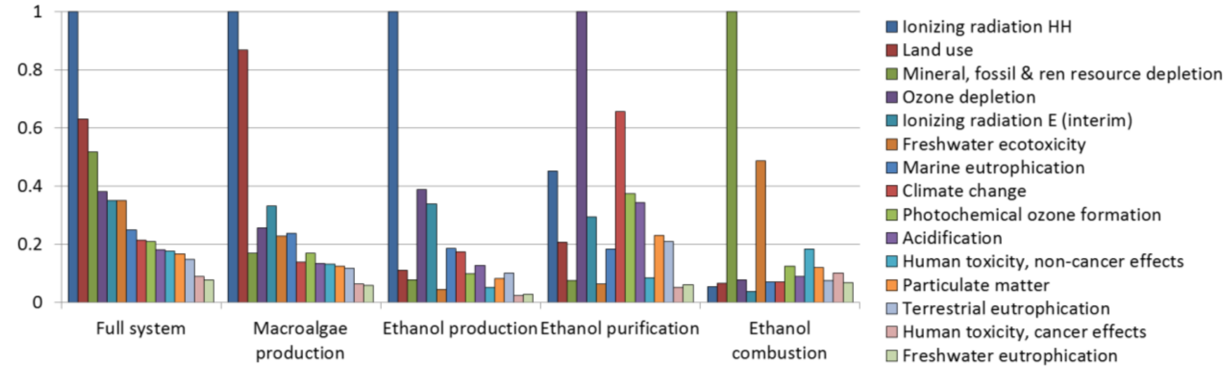
	RI
Macro-algae production subsystem	2.71×10^{-4}
Ethanol production subsystem	7.09×10^{-3}
Ethanol purification subsystem	2.63×10^{-3}
Ethanol combustion subsystem	2.32×10^{-5}
Full system	7.75×10^{-5}

Looking at the RIs of impact categories (see Figure 31), similar trends than the ones observed for global RIs are obtained: ethanol production and purification have very high RIs compared to the other two steps and to the entire LCI result (Figure 31.a). The three most representative impact categories for ethanol production are the two ionizing radiations and ozone depletion. This subsystem has a very different elementary flow pattern compared to the entire LCI result. The potential diminution of the LCA contribution of this particular subsystem would have to be carried out through these three impact categories.

Production of algae obtains similar RI results compared to the entire LCI result (Figure 31.b): ionizing radiation and land use are the most representative impact categories. They are the most suitable impact categories to focus on in order to decrease its LCA contribution. However, ethanol purification and combustion obtain very different RI trends compared to the entire LCI result: ionizing radiation HH is not put forward by our methodology.



a)



b)

Figure 31. a) RI results of the ILCD impact categories (ranking by decreasing RIs of the whole LCI result). **b)** Normalization by the highest RI is applied for each LCI result due to the different magnitude.

Globally, analysing impact category RIs of subsystem put forward the same impact categories that the most representative of the entire LCI result. Magnitudes of the RIs are however deeply modified from a subsystem to another due to different elementary flow patterns. Climate change occupies a singular position by being at the 8th position for the entire LCI result and being ranked second most representative impact category for the ethanol purification.

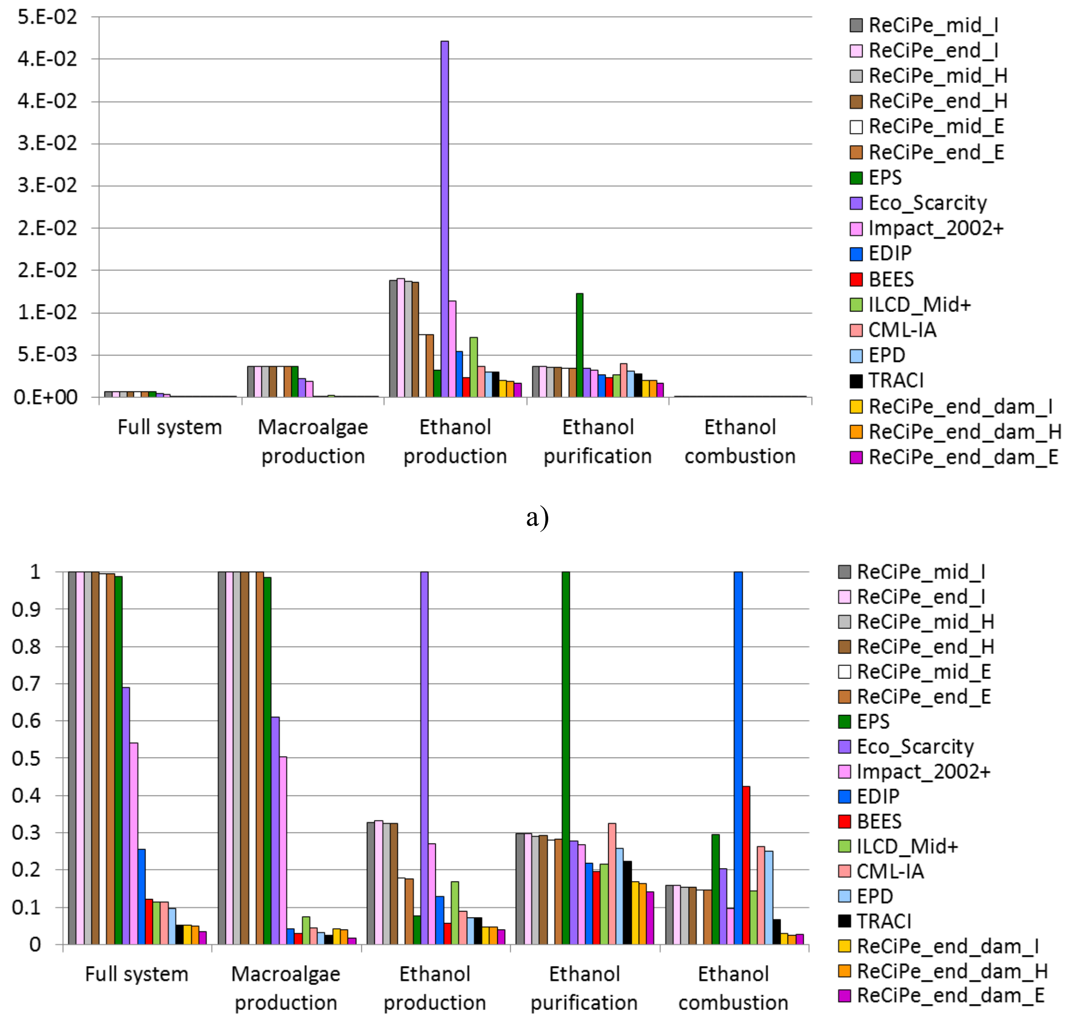
Macro-algae is the main contributive step of the whole system for most of the impacts (Figure 29), but it is not the best represented by ILCD (Figure 31.a). This points out the need of focusing the attention in this step for the improvement of the system and of the assessment.

Considering the ILCD method, the eight impact categories that best represent the environmental issues of the studied system and its subsystems are: ionizing radiation HH, land use, resource depletion, ozone depletion, ionizing radiation E, freshwater ecotoxicity, marine eutrophication and climate change. The interpretation and the ecodesign improvement should preferentially be focused on this subset of the ILCD method.

5.3.2.3. LCIA methods screening

The ILCD method was selected by the goal and scope of the LCA study. We here explore if other classic LCIA methods best represent the LCI and tackle differently the elementary flows patterns of the studied LCI result and its four subsystems. Results of the global RI of LCIA methods are presented in Figure 32.

RIs of the full system are quite low comparing to its subsystems as it was observed for ILCD in part 5.3.2.2. Splitting subsystems allows revealing environmental flow patterns specific of the different steps. Proximities of LCIA methods regarding these subsystems are very different. While studying the entire LCI result would be more relevant with a ReCiPe method, the three last subsystems are putting forward other LCIA method: Ecological Scarcity, EPS and EDIP.



a)

b)

Figure 32. a) RI results of the classic LCIA methods (ranking by decreasing RIs of the whole LCI result). **b)** Normalization by the highest RI is applied for each LCI result due to the different magnitude.

Screening of impact category RIs for the entire system and the four sub-systems is proposed in Annex D – 2. Urban land occupation is the impact category that provides the larger part of RI values of ReCiPe methods. Raceways are modelled to occupy industrial area, the aggregated entire LCI use this elementary flow with high intensity and this impact category considered this dimension with high priority. This land use impact category is more specific than the one belonging to the ILCD methods and it targets intense elementary flows of our LCI result. In addition to the land use issue assessed by several categories, toxicities and ionizing radiations impacts are the other representative environmental issues for this LCI result. This screening could be a tool to inform practitioners that on impact category from other LCIA methods; their LCI results are well represented in term of the elementary flow pattern and the critical dimension of the concerned impact category.

5.4. Conclusions

The environmental hotspots of the production of ethanol from onshore cultivated seaweed were assessed using the LCA methodology. The study reveals that the main contributive step was the algae production on almost all impact categories. It is through its land occupation and its electricity consumption that this step impact on the environment. Yield growth of the studied algae and its cultivation system were the main parameters that could trigger a diminution of the environmental burden of the values chain.

The second objective of this study was to apply an innovative measurement, the RI, to assess the relevance of the environmental indicators used by a LCA. This measurement put forward ionizing radiations, land use and resource depletion as the most representative impact categories of this LCI result. Classic environmental study of transport system always focuses on climate change, fossil fuel depletion and particulate matter issues. However, contextualizing our LCI results within the frame of a large database, the main environmental concerns of our system were on different one. This study case shows the great interest that this methodology could provide to LCA practitioners to support them on eco-design projects.

Chapter 6: General discussion and conclusion

Contents of Chapter 6

The major aim of this thesis was to develop metrics to assess the relevance of a LCIA method and/or a subset of impact categories with respect to the studied systems. The objective was to fully tackle impact categories to the ISO requirement that requests that a "comprehensive set of environmental issues related to the product system" should be analysed. The work leads to the formalization of the LCA framework from a geometric viewpoint and the development of a Representativeness Index per LCIA method and impact category. Neither the scientific nor the environmental relevance of the LCIA method models is assessed here but the approach shows how the LCI result information is caught by the LCIA. In this chapter, it is proposed to review the outcomes of the thesis, to point out their potentials and limitations, and to guide future research efforts to improve and deepen the exploratory approaches developed.

6.1. Main outcomes of the thesis

There were two kinds of outcomes regarding the developed RI measurement: the approach principles and the corresponding practical aspects.

6.1.1. Methodological outcomes

First, the study provides an operational methodology to assess the appropriateness of LCIA method and impact categories while carrying out a LCA (Chapter 2 and 3). This methodology is based on a geometric formalization of the LCA framework. Indeed with a norm and a direction, LCI results and impact categories are considered as vector and can be localized in the same vector space. The LCIA phase of a LCI result is then a classic scalar product and can be visualized with an orthogonal projection. The developed RI measurement relies on the angular distance observed between a LCI result vector and each impact categories, or between a LCI result vector and a multi-dimensional sub-space generated by a set of impact categories. The relevance of indicators used to study an environmental profile can be compared with the RI measurement.

Environmentally critical dimensions are also put forward for all possible impact categories. Then, the developed angular measurement provides an interesting insight on the elementary flows intensity over the critical dimensions determined for the impact category (and subsequently the critical dimensions of the corresponding LCIA method). The standardization procedure determines the elementary flow intensities of each LCI by confronting it with the frame of reference of the LCI database context (a set of LCI result representing the "world" through the modelled activities). The critical dimensions therefor reveal the main problematic dimensions, according to the "world" representation, regarding the modelled environmental mechanisms. By providing additional information based on LCI results, justifications towards the choice of a LCIA method and its decorrelated impact categories can rely on RIs. This innovative methodology assists the practitioner's knowledge by giving an objective overview of his LCI results regarding the human activities modelled and regarding the critical dimensions of each impact categories.

6.1.2. Practical results

Secondly, the main practical outcome of the thesis is an operational tool written in Python 3.6 for RI calculation. The corresponding code is made available from an online deposit (Chapter 3). It allows LCA practitioners to calculate RIs for their own LCI result (ecoinvent 3.1, at point of substitution, for this first version, next improvements should increase the number of databases).

Other practical outcomes have been obtained by confronting the measurement to large sets of LCI results (Chapter 4). By exploring RI results among homogeneous sets of LCI results grouped by their field of activity, it shows contrasted representativeness results of LCIA methods and impact categories. Results are particularly interesting for impact categories that are known to endure environmental pressure from specific fields of activity, and then that are put forward by the RI measurement. For instance, land use, eutrophications and acidification were determined as the best representative impact categories for agriculture and forestry products while climate change, photochemical ozone formation and acidification seemed to be the most relevant impact categories for electricity power generation processes. The RI gives an objective justification to emphasis interpretation of LCA results on some environmental issues by field of study.

Finally, the RI methodology is applied in Chapter 5 on a case study from the Green AlgOhol project: the modelling of a biofuel production from cellulosic macro-algae. First, an environmental contribution analysis is presented. Then, RI analyses of the entire values chain complete the study and investigation of RIs of four sub-parts of the LCI result lead to three main impact categories (ionizing radiation human health, land use and resource depletion) potentially complemented with five others. A screening of RI results (global RIs of LCIA methods and RIs of impact categories) is finally achieved to prospect RIs on other LCIA methods. This shows how RI contributes to an ecodesign approach by adding information on the relevance of assessment criteria for the improvement process.

6.2. Limitations and perspectives of the Representativeness Index

6.2.1. Standardization

As for the most of quantitative multicriteria approaches, the variability of studied dimensions, in term of units and magnitudes, forces to free of them by standardization. The Representativeness methodology presented here therefore depends on standardization by the geometrical mean determined over an entire database. Due to disparities observed among the number of LCI results per field of activity (for instance ecoinvent database has 2,788 LCI results for the electricity power generation and only 280 LCI results for the mining and quarrying field), the standardized elementary flows are obviously oriented according to the features of the most represented fields of activity. Because of some sectors are overrepresented in the database compared to the "real world", the standardization procedure in the RI computation involves that the geometric means of elementary flows do not truly reflect the real elementary flow trends of all the interventions of the techno-sphere with the environment.

Regarding this limit, several research perspectives can be suggested:

- Suppressing overlaps among products can be a first way to limit the number of LCI results within overrepresented fields. Indeed, very similar LCI results (electricity productions from coal from different countries, chemical products with very similar process or modelled with the same proxies...) are present in LCI results databases and might perturb elementary flow trends;
- Standardization using data from input-output databases could also overcome this issue (e.g. EXIOBASE for I-O table with environmental data). Market information between sectors of activity could be used to "weight" them in the standardization procedure. The RI of a LCI result will then face its elementary flow intensities in relation to the territory to which it belongs to and regarding the local environmentally critical dimensions;
- The standardization procedure could also be carried out using elementary flow trends from fields of activity. The issues raised by the number of LCI results per field might be overcome this way if the number of LCI results per field still allows determining a representative geometric mean. However, a standardization intra-field of activity only make LCI result distinguished from their field; inter-field comparison cannot be done. This way, RIs might respond to another specific research question.

6.2.2. Decorrelation

The algorithm of decorrelation proposed in Chapter 3 presents some limitations. Indeed, to deal with overrepresentation and underrepresentation issues, the procedure focuses on the impact category level which generates artifacts and inconsistencies within the decorrelated RIs. Impact categories that are not linked through the dimensions that trigger a potential representation issue might in fact be affected by the decorrelation. To avoid this kind of inconsistency, sharing of the redundant information could be manage by focusing further developments at the dimension level.

6.2.3. Regionalization, variability and other perspectives

Facing the development of the regionalization of LCI results and LCIA methods, LCA data structure might be deeply affected in the future. Detailed data at regional level can multiply the number of dimensions that have to be managed (regionalization involves potential different CFs per substance, compartment and sub-compartment). Obviously, the studied vector space will be larger. Such modifications of the vector space will lead to adapt the RI methodology. The “curse of dimensionality” associated with high-dimensional spaces (Leskovec et al., 2014), which manifests itself by having almost any two vectors to be almost orthogonal, may bring unintuitive RI results. The very low RI results that are currently obtained (from 10^{-2} to 10^{-5}) is already a consequence of the high number of dimensions of the LCA vector space.

When carrying a LCA study, LCI result and elementary flow variabilities and uncertainties can be described. Those variabilities can generate a huge number of different LCI results. The current RI methodology developed in this PhD work didn’t face the issue of variability in LCA and how to take it into account from an operational point of view. However, the variability observed for a given elementary flow over a database is often higher than the variability of this elementary flow determined for a given LCI result. The RI results obtained for a large set of LCI results (whole database or fields of activity) could then not be deeply affected by taking into account the variability of the LCI results. Moreover, RI values of one LCI result can be determined for extreme bounds of the variability of its elementary flows. The link between the variability and the variation of the RI should still be investigated in details.

The direct implementation within LCA dedicated software, the use of different databases and the multiple versions of those databases (which imply a dedicated ad hoc standardization process), but also inconsistencies in the nomenclatures and the structures of the different databases, are practical limitations for the full operationalization of the methodology. The current Python implementation can facilitate the future use of the code given that it is a free license language that is already used in other LCA framework (e.g. Brightway2).

Concerning LCI results databases, the RI methodology has to be tested on other versions of the ecoinvent database and other LCI results databases. Comparing RI results from different databases could guide LCA practitioners on a specific database; even if this choice would still be mainly led by the different rules supervise the development of a database (as for example the system boundaries rules regarding the co-product management).

Finally, this approach could initiate screening of impact categories from up-to-date LCIA methods to generate composite LCIA methods per LCI result. This perspective would have to deal with orthogonalization issues and focus on the complementarity of impact categories to limit representativeness issues among the selected ones. Moreover, the number of impact categories per optimized subsets could be challenging to determine. Specific default lists of impact categories could be proposed per fields of activity through such global analysis of a database.

6.3. General conclusion

Selection of a LCIA method and relevant impact categories for decision support is one of the decisive steps when assessing the environmental burden of human activities with the LCA framework. The selection has to be taken during the goal and scope definition phase and a focus on several impact category results can be done during the interpretation phase. Having an overview of LCI result database, this PhD thesis proposed to question the relevance of a chosen LCIA method and the different impact categories with the development of an innovative metric. This work was led by the following general research question: "By exploring LCI results through their standardized elementary flow trends, is it possible to assess by a systematic approach the relative relevance of LCIA methods and their respective impact categories for LCA studies?"

Using LCI results and a geometric formalization of the LCA methodology, the theoretical basis of the RI measurement was developed in Chapter 2. The RI is an angular distance between a LCI result and a LCIA method. The relevance of LCIA methods was analysed to support LCA practitioner decision. To illustrate the feasibility of such a procedure, the RI measurement was applied on four electricity mix productions case studies. LCIA methods were then discriminate regarding their RI.

The Chapter 3 deepened the analysis at the impact category level to screen, for a LCI result, which indicators are worthwhile focusing on within a LCIA method. A comparative LCA study could then benefit from the RI measurement when interpreting LCIA results. Correlation among impact categories raised representativeness issues that were resolved with the development of an orthogonalization algorithm. A python package was also developed in parallel of this Chapter to provide an operational tool for LCA practitioners.

Finally, Chapter 4 and 5 explored the RI measurement possibilities over a wide range of LCI results segregated by their field of activity and over a case study obtained from the Green AlgOhol project. Field of activity analyses showed different RI trends regarding impact categories that could lead to general guidelines. Splitting an entire LCI result from its main values chain steps uncovers that different impact categories could be focused on for each of them.

Chapter 6 aimed at proposing possible routes for further developments of the RI measurement. LCA practitioners could benefit from such a decision tool but its appropriation still faces challenges.

LCA is a multicriteria decision support. If many works deal with the choice of the indicators (to avoid redundancy, to simplify the decision or to facilitate the interpretation of results), very few studies are focused on the representativeness of the inventory. The questions “What is the part of the initial information that I assess in my analysis?” and “How the impact categories are relevant in front of the technical system?” are issues that are poorly addressed in LCA studies. The RI measurement defined in this PhD provides objective and quantitative answers to these questions and contribute to a more efficient interpretation of LCA results.

One of the great features of the LCA approach is the structuration of the environmental assessment process. The environmental concerns of a human activity are tackled through two aspects: practitioner models activities (LCI: procedure to obtain LCI results) and methods developers provide assessment tools (LCIA methods) for environmental purposes. The work presented in this PhD contributes to a better consistency between these two steps to ensure an efficient assessment.

References

Aitken, D., Bulboa, C., Godoy-Faundez, A., Turrion-Gomez, J.L., Antizar-Ladislao, B., 2014. Life cycle assessment of macroalgae cultivation and processing for biofuel production. J. Clean. Prod. 75, 45–56. https://doi.org/10.1016/j.jclepro.2014.03.080

Alvarado-Morales, M., Boldrin, A., Karakashev, D.B., Holdt, S.L., Angelidaki, I., Astrup, T., 2013. Life cycle assessment of biofuel production from brown seaweed in Nordic conditions. Bioresour. Technol. 129, 92–99. https://doi.org/10.1016/j.biortech.2012.11.029

Aresta, M., Dibenedetto, A., Barberio, G., 2005. Utilization of macro-algae for enhanced CO2 fixation and biofuels production: Development of a computing software for an LCA study. Fuel Process. Technol. 86, 1679–1693. https://doi.org/10.1016/j.fuproc.2005.01.016

Arfken, G.B., Weber, H.J., 2012. Mathematical Methods for Physicists. Academic Press.

Bare, J., 2011. TRACI 2.0: the tool for the reduction and assessment of chemical and other environmental impacts 2.0. Clean Technol. Environ. Policy 13, 687–696. https://doi.org/10.1007/s10098-010-0338-9

Bare, J.C., Gloria, T.P., 2006. Critical Analysis of the Mathematical Relationships and Comprehensiveness of Life Cycle Impact Assessment Approaches. Environ. Sci. Technol. 40, 1104–1113. https://doi.org/10.1021/es051639b

Basson, L., Petrie, J.G., 2007. An integrated approach for the consideration of uncertainty in decision making supported by Life Cycle Assessment. Environ. Model. Softw. 22, 167–176. https://doi.org/10.1016/j.envsoft.2005.07.026

Bava, L., Sandrucci, A., Zucali, M., Guerci, M., Tamburini, A., 2014. How can farming intensification affect the environmental impact of milk production? J. Dairy Sci. 97, 4579–93. https://doi.org/10.3168/jds.2013-7530

Bixler, H.J., Porse, H., 2011. A decade of change in the seaweed hydrocolloids industry. J. Appl. Phycol. 23, 321–335. https://doi.org/10.1007/s10811-010-9529-3

Brockmann, D., Pradinaud, C., Champenois, J., Benoit, M., Hélias, A., 2015. Environmental assessment of bioethanol from onshore grown green seaweed. Biofuels, Bioprod. Biorefining. https://doi.org/10.1002/bbb.1577

Cappelli, A., Gigli, E., Romagnoli, F., Simoni, S., Blumberga, D., Palerno, M., Guerriero, E., 2015. Co-digestion of Macroalgae for Biogas Production: An LCA-based Environmental Evaluation. Energy Procedia 72, 3–10. https://doi.org/10.1016/j.egypro.2015.06.002

Chen, X., Samson, E., Tocqueville, A., Aubin, J., 2015. Environmental assessment of trout farming in France by life cycle assessment : using bootstrapped principal component analysis to better de fi ne system classi fi cation. J. Clean. Prod. 87, 87–95. https://doi.org/10.1016/j.jclepro.2014.09.021

Collet, P., Hélias, A., Lardon, L., Steyer, J.-P., Bernard, O., 2015. Recommendations for Life Cycle Assessment of algal fuels. Appl. Energy. https://doi.org/10.1016/j.apenergy.2015.03.056

Collet, P., Hélias Arnaud, A., Lardon, L., Ras, M., Goy, R.A., Steyer, J.P., 2011. Life-cycle assessment of microalgae culture coupled to biogas production. Bioresour.

Technol. 102, 207–214. https://doi.org/10.1016/j.biortech.2010.06.154

Cortés-Borda, D., Guillén-Gosálbez, G., Esteller, L.J., 2013. On the use of weighting in LCA: Translating decision makers' preferences into weights via linear programming. Int. J. Life Cycle Assess. 18, 948–957. https://doi.org/10.1007/s11367-012-0540-6

Davis, R., Tao, L., Tan, E.C.D., Biddy, M.J., Beckham, G.T., Scarlata, C., Ross, J., Lukas, J., Knorr, D., Schoen, P., 2013. Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons : Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Biological Conversion of Sugars to Hydrocarbons Process Design and Economics for the Conversion. https://doi.org/10.2172/1107470

De Saxcé, M., Rabenasolo, B., Perwuelz, A., 2014. Assessment and improvement of the appropriateness of an LCI data set on a system level - Application to textile manufacturing. Int. J. Life Cycle Assess. 19, 950–961. https://doi.org/10.1007/s11367-013-0679-9

Dreyer, L.C., Niemann, A.L., Hauschild, M.Z., 2003. Comparison of Three Different LCIA Methods: EDIP97, CML2001 and Eco-indicator 99. Int. J. Life Cycle Assess. 8, 191–200. https://doi.org/10.1007/BF02978471

Dunn, J.B., Mueller, S., Wang, M., Han, J., 2012. Energy consumption and greenhouse gas emissions from enzyme and yeast manufacture for corn and cellulosic ethanol production. Biotechnol. Lett. 34, 2259–2263. https://doi.org/10.1007/s10529-012-1057-6

EC-JRC, 2011. International Reference Life Cycle Data System (ILCD) Handbook: Recommendations for Life Cycle Impact Assessment in the European context, First Edit. ed. Institute for Environment and Sustainability. https://doi.org/10.278/33030

EC-JRC, 2010a. International Reference Life Cycle Data System (ILCD) Handbook: General guide for Life Cycle Assessment - Detailed guidance, First Edit. ed, European Commission. Institute for Environment and Sustainability. https://doi.org/10.2788/38479

EC-JRC, 2010b. International Reference Life Cycle Data System (ILCD) Handbook: Analysing of existing Environmental Impact Assessment methodologies for use in Life Cycle Assessment, First Edit. ed, European Commission. Institute for Environment and Sustainability.

Esnouf, A., Latrille, É., Steyer, J.-P., Helias, A., 2018. Representativeness of environmental impact assessment methods regarding Life Cycle Inventories. Sci. Total Environ. 621, 1264–1271. https://doi.org/10.1016/j.scitotenv.2017.10.102

EXIOBASE [WWW Document], n.d. URL https://www.exiobase.eu

Frischknecht, R., Sybille, B.K., 2013. Swiss Eco-Factors 2013 according to the Ecological Scarcity Method. Methodological fundamentals and their application in Switzerland. Environmental studies no. 1330; Federal Office for the Environment, Bern.

Gentle, J.E., 2007. Matrix Algebra, Springer Texts in Statistics. Springer New York, New York, NY. https://doi.org/10.1007/978-0-387-70873-7

Gniazdowski, Z., 2013. Geometric interpretation of a correlation. Zesz. Nauk. Warsz. Wyższej Szk. Inform. 7, 27–35.

Goedkoop, M., Heijungs, R., Huijbregts, M., Schryver, A. De, Struijs, J., Zelm, R. Van, 2009. ReCiPe 2008: A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level. https://doi.org/10.029/2003JD004283

Guinée, J.B., 2015. Selection of Impact Categories and Classification of LCI Results to Impact Categories, in: Hauschild, M.Z., Huijbregts, M.A.J. (Eds.), Life Cycle Impact Assessment. Springer Netherlands, pp. 17–37. https://doi.org/10.1007/978-94-017-9744-3_2

Guinée, J.B., Gorre, M., Heijungs, R., Huppes, G., Kleijn, R., van Oers, L., Wegener Sleeswijk, A., Suh, S., Udo de Haes, A.H., de Bruijn, H., van Duin, R., Huijbregts, M.A.J., 2001. Handbook on Life Cycle Assessment, Operational guide to the ISO standards Volume 1, 2a, 2b and 3.

Hauschild, M., Potting, J., 2005. Spatial differentiation in Life Cycle impact assessment - The EDIP2003 methodology. Report for the Danish Environmental Protection Agency.

Hauschild, M.Z., Goedkoop, M., Guinée, J., Heijungs, R., Huijbregts, M., Jolliet, O., Margni, M., De Schryver, A., Humbert, S., Laurent, A., Sala, S., Pant, R., 2013. Identifying best existing practice for characterization modeling in life cycle impact assessment. Int. J. Life Cycle Assess. 18, 683–697. https://doi.org/10.1007/s11367-012-0489-5

Heijungs, R., 2017. Comment on "Resource Footprints are Good Proxies of Environmental Damage." Environ. Sci. Technol. 51, 13054–13055. https://doi.org/10.1021/acs.est.7b04253

Heijungs, R., Suh, S., 2002. The Computational Structure of Life Cycle Assessment. Eco-Efficiency in Industry and Science, Vol. 11. Kluwer Academic Publishers.

Hoekstra, A.Y., Wiedmann, T.O., 2014. Humanity's unsustainable environmental footprint. Science (80-.). 344, 1114–1117. https://doi.org/10.1126/science.1248365

Hughes, A.D., Kelly, M.S., Black, K.D., Stanley, M.S., 2012. Biogas from Macroalgae: Is it time to revisit the idea? Biotechnol. Biofuels 5, 1–7. https://doi.org/10.1186/1754-6834-5-86

Huijbregts, M.A.J., Rombouts, L.J.A., Hellweg, S., Frischknecht, R., Hendriks, A.J., van de Meent, D., Ragas, A.M.J., Reijnders, L., Struijs, J., 2006. Is Cumulative Fossil Energy Demand a Useful Indicator for the Environmental Performance of Products ? 40, 641–648. https://doi.org/10.1021/es051689g

Huijbregts, M.A.J., Steinmann, Z.J.N., Elshout, P.M.F., Stam, G., Verones, F., Vieira, M., Zijp, M., Hollander, A., van Zelm, R., 2016. ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. Int. J. Life Cycle Assess. 1–16. https://doi.org/10.1007/s11367-016-1246-y

Humbird, D., Davis, R., Tao, L., Kinchin, C., Hsu, D., Aden, A., 2011. Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol.

ISO, 2006a. ISO 14040: Environmental Management - Life Cycle Assessment Principles and Framework. Geneva, Switzerland.

ISO, 2006b. ISO 14044: Environmental Management - Life Cycle Assessment Requirements and Guidelines. Geneva, Switzerland.

Jolliet, O., Antón, A., Boulay, A.-M., Cherubini, F., Fantke, P., Levasseur, A., McKone, T.E., Michelsen, O., Milà i Canals, L., Motoshita, M., Pfister, S., Verones, F., Vigon, B., Frischknecht, R., 2018. Global guidance on environmental life cycle impact assessment indicators: impacts of climate change, fine particulate matter formation, water consumption and land use. Int. J. Life Cycle Assess. 1–19. https://doi.org/10.1007/s11367-018-1443-y

Jolliet, O., Margni, M., Charles, R., Humbert, S., Payet, J., Rebitzer, G., Rosenbaum, R., 2003. IMPACT 2002+: A new life cycle impact assessment methodology. Int. J. Life Cycle Assess. 8, 324–330. https://doi.org/10.1007/BF02978505

Jungbluth, N., Chudacoff, M., 2007. Life cycle inventories of bioenergy. Final Rep. ecoinvent ….

Langlois, J., Sassi, J.-F., Jard, G., Steyer, J.-P., Delgenes, J.-P., Hélias, A., 2012. Life cycle assessment of biomethane from offshore-cultivated seaweed. Biofuels, Bioprod. Biorefining 6, 387–404. https://doi.org/10.1002/bbb.1330

Laurent, A., Clavreul, J., Bernstad, A., Bakas, I., Niero, M., Gentil, E., Christensen, T.H., Hauschild, M.Z., 2014. Review of LCA studies of solid waste management systems – Part II: Methodological guidance for a better practice. Waste Manag. 34, 589–606. https://doi.org/10.1016/j.wasman.2013.12.004

Lautier, A., Rosenbaum, R.K., Margni, M., Bare, J., Roy, P.-O., Deschênes, L., 2010. Development of normalization factors for Canada and the United States and comparison with European factors. Sci. Total Environ. 409, 33–42. https://doi.org/10.1016/j.scitotenv.2010.09.016

Leskovec, J., Rajaraman, A., Ullman, J., 2014. Mining of Massive Datasets. Stanford Computer Science course CS246.

Meadows, D.H., Meadows, D.L., Randers, J., Behrens, W.W., 1972. The Limits to Growth, Universe b. ed. https://doi.org/10.1111/j.1752-1688.1972.tb05230.x

Mendoza Beltran, A., Prado, V., Font Vivanco, D., Henriksson, P.J.G., Guinée, J.B., Heijungs, R., 2018. Quantified Uncertainties in Comparative Life Cycle Assessment: What Can Be Concluded? Environ. Sci. Technol. acs.est.7b06365. https://doi.org/10.1021/acs.est.7b06365

Monteiro, H., Freire, F., 2012. Life-cycle assessment of a house with alternative exterior walls: Comparison of three impact assessment methods. Energy Build. 47, 572–583. https://doi.org/10.1016/j.enbuild.2011.12.032

Moreno Ruiz, E., Weidema, B.P., Bauer, C., Nemecek, T., Vadenbo, C.O., Treyer, K., Wernet, G., 2013. Documentation of changes implemented in ecoinvent Data 3.0. Ecoinvent Report 5 (v4); St. Gallen: The ecoinvent Centre.

Mouron, P., Nemecek, T., Scholz, R.W., Weber, O., 2006. Management influence on environmental impacts in an apple production system on Swiss fruit farms: Combining life cycle assessment with statistical risk assessment. Agric. Ecosyst. Environ. 114, 311–322. https://doi.org/10.1016/j.agee.2005.11.020

Mu, D., Seager, T., Rao, P.S., Zhao, F., 2010. Comparative life cycle assessment of lignocellulosic ethanol production: Biochemical versus thermochemical conversion. Environ. Manage. 46, 565–578. https://doi.org/10.1007/s00267-010-9494-2

Mutel, C., 2017. Brightway: An open source framework for Life Cycle Assessment. J. Open Source Softw. 2, 236. https://doi.org/10.21105/joss.00236

NIST, 2007. BEES 4.0: Building for Environmental and Economic Sustainability.

Technical Manual and User Guide.

Owsianiak, M., Laurent, A., Bjørn, A., Hauschild, M.Z., 2014. IMPACT 2002+, ReCiPe 2008 and ILCD’s recommended practice for characterization modelling in life cycle impact assessment: a case study-based comparison. Int. J. Life Cycle Assess. 19, 1007–1021. https://doi.org/10.1007/s11367-014-0708-3

Pandey, A., Lee, D.J., Chisti, Y., Soccol, C.R., 2014. Biofuels from algae, Elsevier S. ed. Elsevier B.V.

Pascual-González, J., Guillén-Gosálbez, G., Mateo-Sanz, J.M., Jiménez-Esteller, L., 2016. Statistical analysis of the ecoinvent database to uncover relationships between life cycle impact assessment metrics. J. Clean. Prod. 112, 359–368. https://doi.org/10.1016/j.jclepro.2015.05.129

Pascual-González, J., Pozo, C., Guillén-Gosálbez, G., Jiménez-Esteller, L., 2015. Combined use of MILP and multi-linear regression to simplify LCA studies. Comput. Chem. Eng. 82, 34–43. https://doi.org/10.1016/j.compchemeng.2015.06.002

Perez, F., Granger, B.E., 2007. IPython: A System for Interactive Scientific Computing. Comput. Sci. Eng. 9, 21–29. https://doi.org/10.1109/MCSE.2007.53

Pilicka, I., Blumberga, D., Romagnoli, F., 2011. Life Cycle Assessment of Biogas Production from Marine Macroalgae: a Latvian Scenario. Sci. J. Riga Tech. Univ. Environ. Clim. Technol. 6, 69–78. https://doi.org/10.2478/v10145-011-0010-6

Pizzol, M., Christensen, P., Schmidt, J., Thomsen, M., 2011. Impacts of “metals” on human health: a comparison between nine different methodologies for Life Cycle Impact Assessment (LCIA). J. Clean. Prod. 19, 646–656. https://doi.org/10.1016/j.jclepro.2010.05.007

Pozo, C., Ruíz-Femenia, R., Caballero, J., Guillén-Gosálbez, G., Jiménez, L., 2012. On the use of Principal Component Analysis for reducing the number of environmental objectives in multi-objective optimization: Application to the design of chemical supply chains. Chem. Eng. Sci. 69, 146–158. https://doi.org/10.1016/j.ces.2011.10.018

Prado-Lopez, V., Seager, T.P., Chester, M., Laurin, L., Bernardo, M., Tylock, S., 2014. Stochastic multi-attribute analysis (SMAA) as an interpretation method for comparative life-cycle assessment (LCA). Int. J. Life Cycle Assess. 19, 405–416. https://doi.org/10.1007/s11367-013-0641-x

Qin, Y., Suh, S., 2016. What distribution function do life cycle inventories follow? Int. J. Life Cycle Assess. 1. https://doi.org/10.1007/s11367-016-1224-4

Rack, M., Valdivia, S., Sonnemann, G., 2013. Life Cycle Impact Assessment—where we are, trends, and next steps: a late report from a UNEP/SETAC Life Cycle Initiative workshop and a few updates from recent developments. Int. J. Life Cycle Assess. 18, 1413–1420. https://doi.org/10.1007/s11367-013-0569-1

Rosenbaum, R.K., 2017. Selection of Impact Categories, Category Indicators and Characterization Models in Goal and Scope Definition. Chapter 2: Goal and Scope Definition in Life Cycle Assessment, in: Curran, M. (Ed.), Klöpffer W, Curran MA, Series (Eds) LCA Compendium – The Complete World of Life Cycle Assessment. pp. 63–122. https://doi.org/10.1007/978-94-024-0855-3_1

Schultz-Jensen, N., Thygesen, A., Leipold, F., Thomsen, S.T., Roslander, C., Lilholt, H., Bjerre, A.B., 2013. Pretreatment of the macroalgae Chaetomorpha linum for the production of bioethanol--comparison of five pretreatment technologies. Bioresour. Technol. 140, 36–42. https://doi.org/10.1016/j.biortech.2013.04.060

Seghetta, M., Romeo, D., D'Este, M., Alvarado-Morales, M., Angelidaki, I., Bastianoni, S., Thomsen, M., 2017. Seaweed as innovative feedstock for energy and feed – Evaluating the impacts through a Life Cycle Assessment. J. Clean. Prod. 150, 1–15. https://doi.org/10.1016/j.jclepro.2017.02.022

Steen, B., 1999a. A systematic approach to environmental priority strategies in product development (EPS). Version 2000 – General system characteristics. CPM report 1999:4.

Steen, B., 1999b. Environmental Assessment of Products and Material Systems A systematic approach to environmental priority strategies in product development (EPS). Version 2000 – General system characteristics. CPM report 1999:5.

Steinmann, Z.J.N., Schipper, A.M., Hauck, M., Giljum, S., Wernet, G., Huijbregts, M.A.J., 2017. Resource Footprints are Good Proxies of Environmental Damage. Environ. Sci. Technol. 51, 6360–6366. https://doi.org/10.1021/acs.est.7b00698

Steinmann, Z.J.N., Schipper, A.M., Hauck, M., Huijbregts, M.A.J., 2016. How Many Environmental Impact Indicators Are Needed in the Evaluation of Product Life Cycles? Environ. Sci. Technol. 50, 3913–3919. https://doi.org/10.1021/acs.est.5b05179

Téno, J.-F. Le, 1999. Visual data analysis and decision support methods for non-deterministic LCA. Int. J. Life Cycle Assess. 4, 41–47. https://doi.org/10.1007/BF02979394

Udo de Haes, A.H., Jolliet, O., Finnveden, G., Hauschild, M., Krewit, W., Muller-Wenk, R., 1999. Best available practice regarding impact categories and category indicators in life cycle impact assessment. Int. J. Life Cycle Assess. 4, 167–174. https://doi.org/10.1007/BF02979453

United Nation, 2008. International Standard Industrial Classification of All Economic Activities (ISIC), Revision 4.

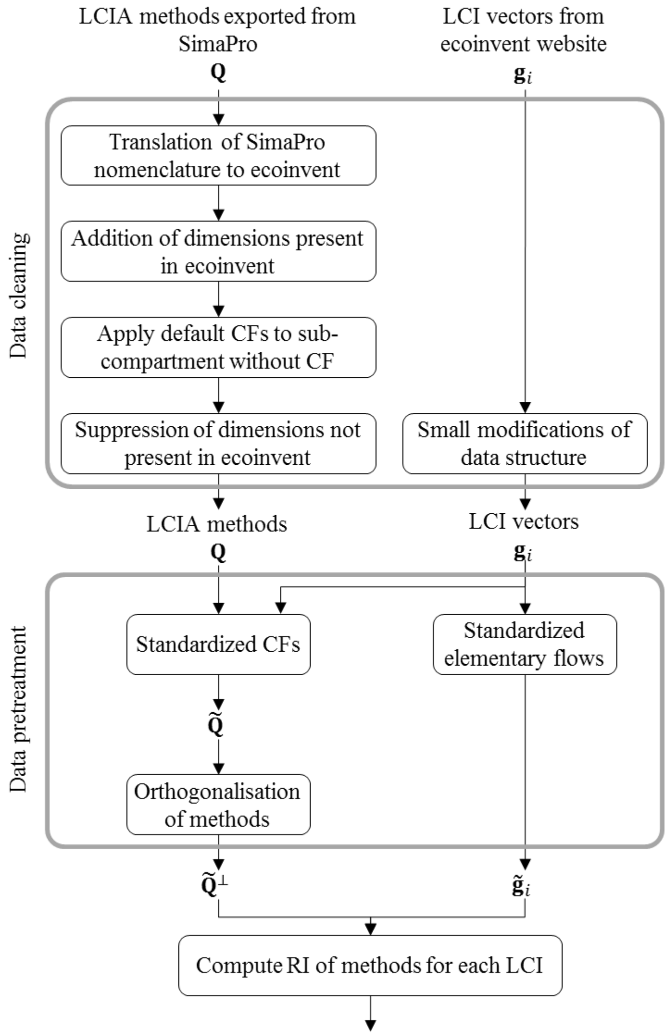
United Nations, 2015. Transforming our world: The 2030 agenda for sustainable development 1–5.

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

Annexes

Contents of Annexes

Annex A: Supplementary Information – Chapter 2



$$RI(\boldsymbol{Q},\boldsymbol{g_i}) = |\cos(\alpha_{\mathbf{Q},i})| = \left|\cos\left(\arcsin\left(\frac{\widetilde{\boldsymbol{g}}_i\widetilde{\boldsymbol{g}}_{i\widetilde{C}^{\perp}}}{\|\widetilde{\boldsymbol{g}}_i\|}\right)\right)\right| = \sqrt{1-\left(\frac{\|\mathbf{g}_i-\mathbf{g}_{i,\mathrm{Q}}\|}{\|\mathbf{g}_i\|}\right)^2}$$

Figure S 1. Schematics of the full procedure, from exportation of data to RI calculation

Data cleaning of LCIA methods takes place in four steps. The first is a translation of the SimaPro nomenclature of elementary flows (substance, compartment and sub-compartment) to the ecoinvent nomenclature. The other three steps are needed in this order to deal with CFs that are only characterized for “unspecified” sub-compartment in SimaPro, while the ecoinvent nomenclature does not have “unspecified” but only the specified sub-compartments.

For example, ecoinvent can have “surface water” and “ocean” sub-compartments for the “water” compartment and no “unspecified” sub-compartment, while an impact category only has CF for the “unspecified” sub-compartment. The procedure will apply the same CF from the “unspecified” to the “surface water” and “ocean” sub-compartments and will delete, at the end, the “unspecified” sub-compartments.

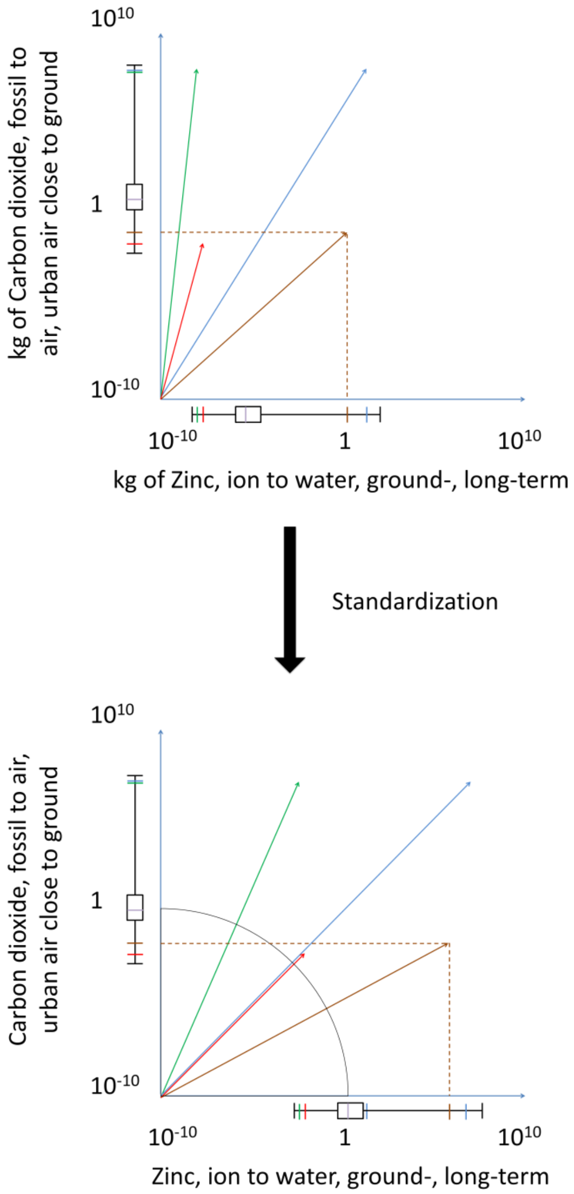


Figure S 2. Standardization of four illustrative LCI results in two dimensions (boxplots show the distribution of the whole database)

The figure illustrates that the existence of different measurement units and orders of magnitude can have consequences on the LCI result vector direction. Standardization brings the boxplots into line and equally discriminates LCIs within the database.

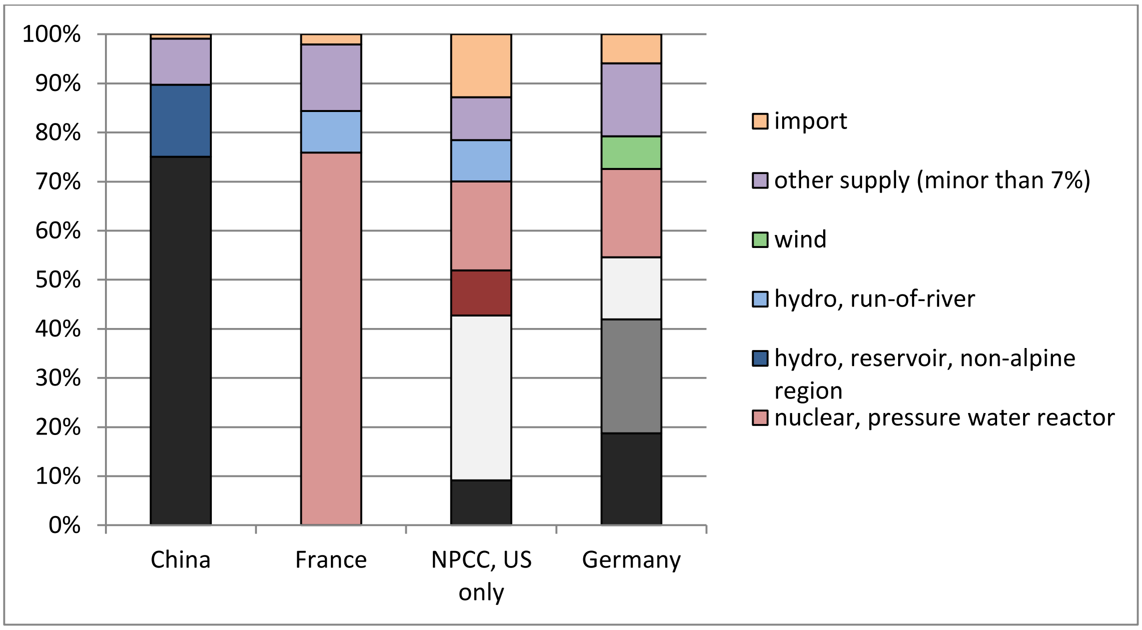


Figure S 3. Electricity mix production from the 4 studied countries. These mixes were extracted from the ecoinvent 3.1“allocation at the point of substitution” version.

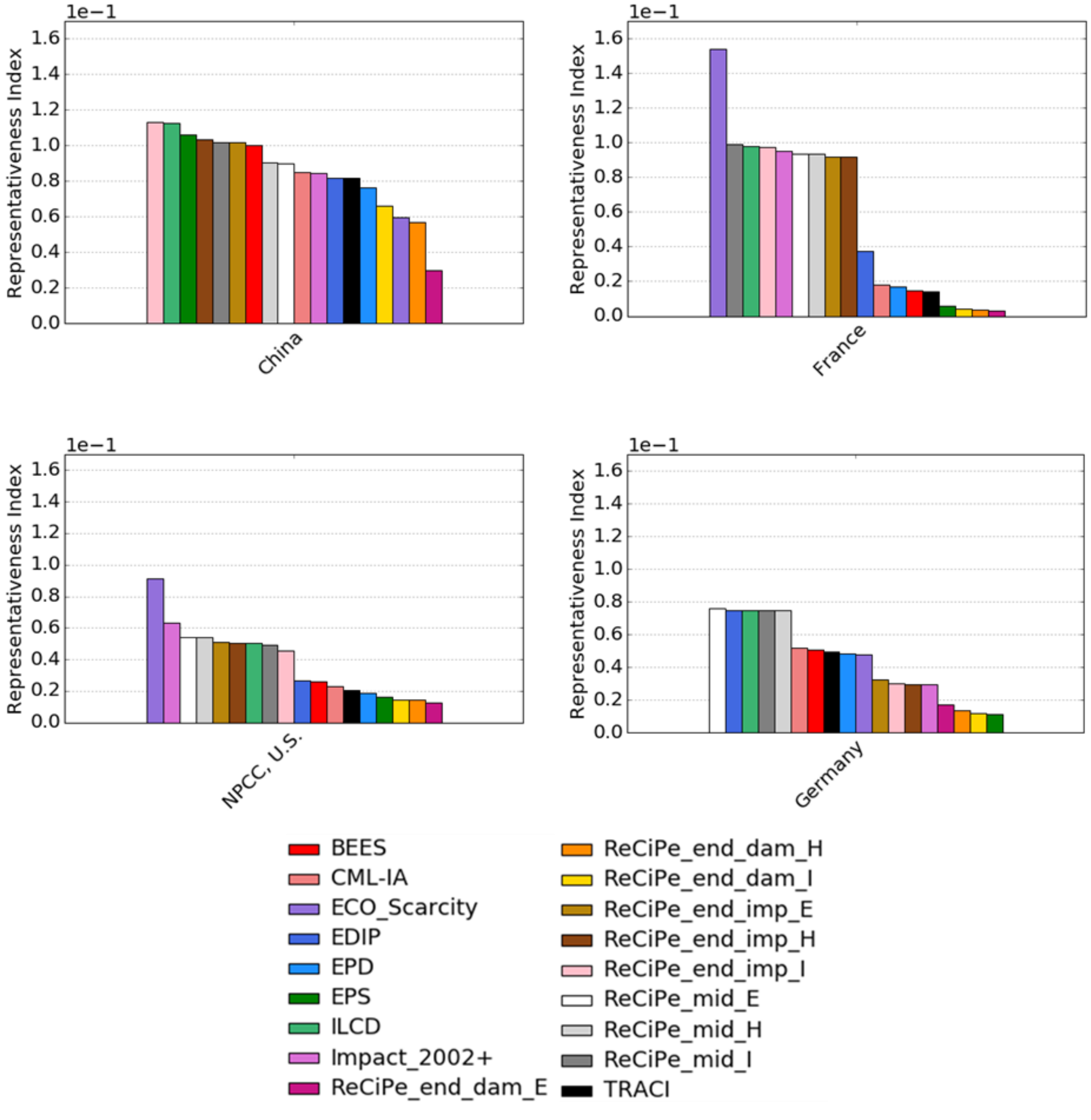


Figure S 4. Representativeness Index (RI) of LCIA methods for the 4 studied electricity mix productions. For each mix production, LCIA methods decrease in order of RIs.

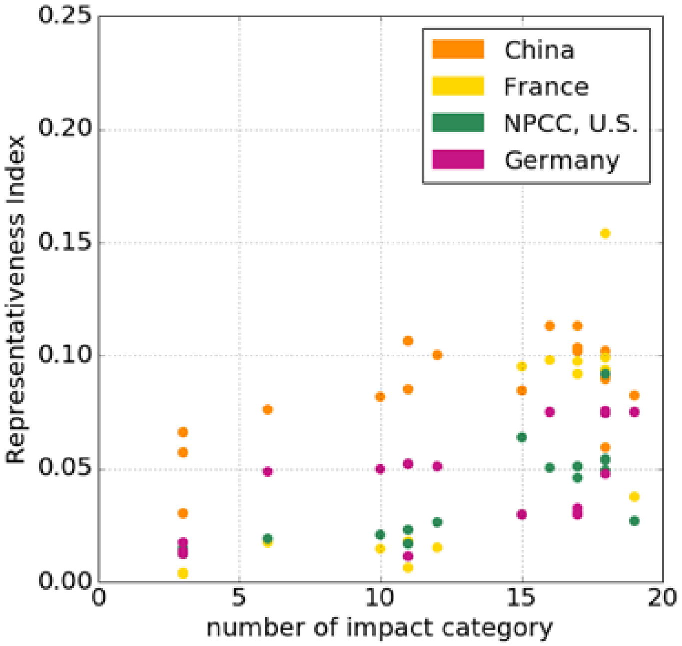


Figure S 5. Relationship between RI scores of the 18 LCIA methods for the 4 studied LCIs and the number of impact category per LCIA method.

Annex B: Supplementary Information – Chapter 3

Annex B-1: Inventory standardization regardless of reference flow

The following development presents the advantages of using the geometric means to standardize elementary flows. The choice of the geometric means is interesting for the calculus of the RI regarding the specific format of the data used. Indeed, each LCI result (which is a compilation of elementary flows) is associated with a reference flow that corresponds to the quantity of product or service provided. Referenced flows are expressed in various units (kg of product, kWh generated, t.km transported…) which obviously raise inconsistency while studying sets of LCI results or a global database. However, using the geometric mean and an angular distance allow obtaining RIs independent from the value of each reference flow.

Let consider a cumulated LCI database DB composed of m LCI results described over n elementary flow dimensions. For homogenisation of elementary flows, the standardization consists here in dividing the elementary flows of each elementary flow by their respective geometric mean.

The expression of the geometric mean G_x over a certain elementary flow x using all the LCI results of the cumulated LCI database DB (with a total of m LCI results) is:

$$G_x = \sqrt[m]{\prod_{i=1}^{m} g_{x,i}} \qquad \text{(SI.1)}$$

To present why the geometric mean is interesting to use regarding the specificity of LCI result data on their reference flow, we consider another cumulated LCI database DB* composed of exactly the same LCI results except for the *"a"* LCI result which is different by its reference flow: it is set δ times higher than in DB. Taking a transportation LCI as an example, this factor could be 1 000 times for this human activity described for 1 t.km (in DB*) instead of 1 kg.km (in DB). All the elementary flows of this LCI are 1 000 higher in DB* than in DB whereas they model the same activity. We have

$$\mathbf{g}_i^* = \mathbf{g}_i \text{ , and } \mathbf{g}_a^* = \delta \times \mathbf{g}_a \qquad \text{(SI.2)}$$

where $i \in \{1, \ldots, m\},\ i \neq a$. The expression of the geometric mean G^*_x for DB* is then:

$$G_x^* = \sqrt[m]{\delta \times g_{x,a}} \times \sqrt[m]{\prod_{\substack{i=1 \\ i \neq a}}^{m} g_{x,i}} \qquad \text{(SI.3)}$$

$$G_x^* = \sqrt[m]{\delta} \times G_x \qquad \text{(SI.4)}$$

Within DB and DB*, a standardized x elementary flow is then:

$$\tilde{g}_{x,i} = \frac{g_{x,i}}{G_x} \text{ , and } \tilde{g}_{x,i}^* = \frac{g_{x,i}}{G_x^*} \qquad \text{(SI.5)}$$

From equation SI.2 and SI.3, we have:

$$\tilde{g}_{x,i}^* = \frac{1}{\sqrt[m]{\delta}} \times \tilde{g}_{x,i} \qquad \text{(SI.6)}$$

The norm of $\tilde{\mathbf{g}}_i^*$ is linked to the norm of $\tilde{\mathbf{g}}_i$ as follows

$$\|\tilde{\mathbf{g}}_i^*\| = \frac{1}{\sqrt[m]{\delta}} \times \|\tilde{\mathbf{g}}_i\| \qquad \text{(SI.7)}$$

Similarly, with the standardized Characterization Factors

$$\tilde{q}_{x,j} = q_{x,j} \times G_x \text{ , and } \tilde{q}_{x,j}^* = q_{x,j} \times G_x^* \qquad \text{(SI.8)}$$

and using equation (SI.4), we obtain the following relations:

$$\tilde{q}_{x,j}^* = \sqrt[m]{\delta} \times \tilde{q}_{x,j}, \text{ and } \left\|\tilde{\mathbf{q}}_j^*\right\| = \sqrt[m]{\delta} \times \left\|\tilde{\mathbf{q}}_j\right\| \qquad \text{(SI.9)}$$

With equation 10, we have the development of $RI\left(\tilde{\mathbf{q}}_j^*, \tilde{\mathbf{g}}_i^*\right)$ using DB*

$$RI\left(\tilde{\mathbf{q}}_j^*, \tilde{\mathbf{g}}_i^*\right) = \left|\frac{\langle \tilde{\mathbf{q}}_j^*, \tilde{\mathbf{g}}_i^* \rangle}{\left\|\tilde{\mathbf{q}}_j^*\right\| \times \left\|\tilde{\mathbf{g}}_i^*\right\|}\right| \qquad \text{(SI.10)}$$

With $\langle \tilde{\mathbf{q}}_j^*, \tilde{\mathbf{g}}_i^* \rangle = \sum_{x=1}^{n} (\tilde{q}_{x,j}^* \times \tilde{g}_{x,i}^*)$ and equations (SI.6-SI.9), this is rewritten

$$RI\left(\tilde{\mathbf{q}}_j^*, \tilde{\mathbf{g}}_i^*\right) = \left|\frac{\sum_{x=1}^{n}\left(\sqrt[m]{\delta} \times \tilde{q}_{x,j} \times \frac{1}{\sqrt[m]{\delta}} \times \tilde{g}_{x,i}\right)}{\sqrt[m]{\delta} \times \left\|\tilde{\mathbf{q}}_j\right\| \times \frac{1}{\sqrt[m]{\delta}} \times \|\tilde{\mathbf{g}}_i\|}\right| \qquad \text{(SI.11)}$$

And finally after simplification

$$RI\left(\tilde{\mathbf{q}}_j^*, \tilde{\mathbf{g}}_i^*\right) = RI\left(\tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_i\right) \qquad \text{(SI.12)}$$

Moreover, concerning the $\mathbf{g}_a$

$$RI\left(\tilde{\mathbf{q}}_j^*, \tilde{\mathbf{g}}_a^*\right) = \left|\frac{\sum_x^n\left(\tilde{q}_{x,j} \times \delta \times \tilde{g}_{x,a}\right)}{\left\|\tilde{\mathbf{q}}_j\right\| \times \delta \times \|\tilde{\mathbf{g}}_a\|}\right| \qquad \text{(SI.13)}$$

which equals to $RI\left(\tilde{\mathbf{q}}_j, \tilde{\mathbf{g}}_a\right)$.

The same reasoning can be easily extended to more than one different reference flows between DB and DB*. This shows that the standardization by the geometric mean allows to RIs being independent of the reference flows used in databases.

Annex B-2: Standardizations and LCI patterns

The aim of Annex B - 1 is to explain the meaning of the standardization. Focus is put on the elementary flow level, which is the core of the information contained by LCI results. Firstly, all data analysis procedures require a pretreatment step to homogenize the data. Each procedure depends on the question and on the structure of the analysed data.
For homogenisation of elementary flows, the standardization consisted in dividing the elementary flows of each dimensions by their respective geometric mean. The set of geometric means summarizes the global trend of the cumulated LCI database over each dimension: it is the average LCI result of a database.

By standardizing each LCI result by the set of geometric means, the dimensions where they are particularly intensive regarding the rest of the LCI results can be revealed. For each standardized LCI result, a division by their norms can be made in order to determine and compare the standardized elementary flows from different LCI results without any influence of their reference flows. In any case, this normalisation is part of the calculus of RIs (cf. equations 4 of the chapter 2 and 3). It is required here for exactly the same reason as the influence of the reference flow value. Standardized elementary flows therefore follow the same numerical range and have a maximal value of 1. The high standardized elementary flows guide the orientation of the LCI result vector. For each LCI result of the cumulated LCI database, we determined the number of different dimensions where the standardized elementary flows allow for 95% of the norm to be reached (i.e. the number of dimensions that assembles the principal information on the direction). We then split the LCI results according to their number of dimensions and plot, with a maximum of 20 dimensions, the Figure S 6. The standardized elementary flow distributions are also presented in Figure S 7.

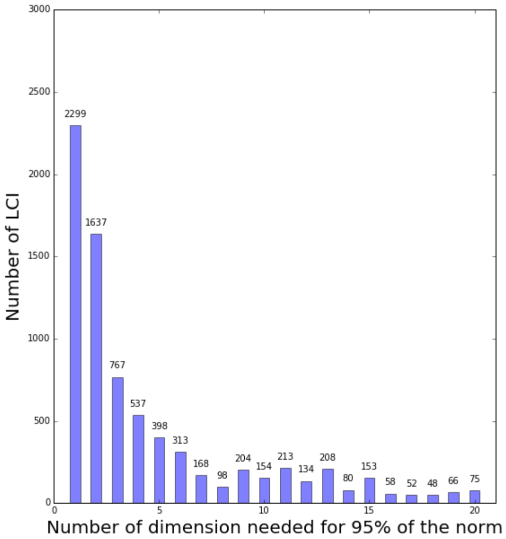


Figure S 6. Number of LCI result per number of dimensions that assemble 95% of their principal information

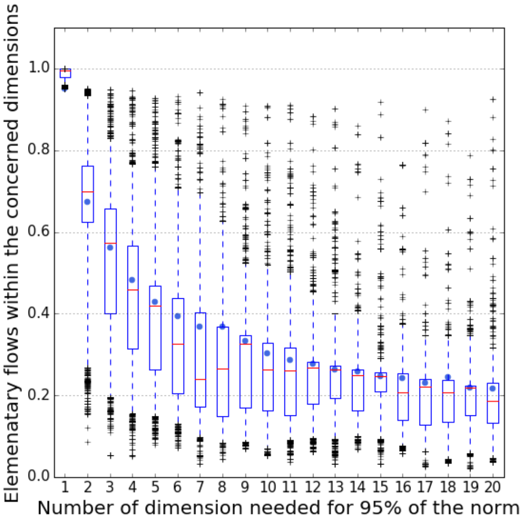


Figure S 7. Distribution of the standardized elementary flows per number of dimensions (for each box plot, the number of data is then "number of dim" multiplied by the "number of LCI result"). The minimal value of the maximal elementary flow is depicted by a blue dot.

These two figures accumulate the results of the standardized elementary flows of 7660 different LCI results. The other LCI results need more than 20 different dimensions to reach 95% of their norm. They reveal flow patterns on LCI results where the two extremes are: either a very intensive LCI result on one precise standardized elementary flow while all the other standardized elementary flows present a very low weight on the norm; or the LCI result information is totally spread out over all the dimensions with equal and relatively low standardized elementary flows. With a database such as ecoinvent 3.1, built with 1727 dimensions, the standardized elementary flows of LCI results that are equally spread over all dimensions have a value of $1/\sqrt{1727} = 2.41 \times 10^{-2}$. Such a LCI result is in fact the standardized average LCI result of the database with, before being standardized, the geometric means as elementary flows. This value is also the minimum value that the highest elementary flow of an LCI result could reach. This LCI result, however is not observed because the maximal number of dimensions needed for 95% of the norm is 640 dimensions. For 2299 LCI results, the main direction of the vectors is dominated by one dimension (Figure S 6). Obviously, Figure S 7 indicates that the values of the standardized elementary flows are above 0.95. Through the value of one elementary flow, these LCI results distinguish themselves significantly, regarding the average LCI result of the database.

Figure S 6 reveals that half of the LCI results of the database only need 5 or less dimensions, to comprise up to 95% of the norm. When more dimensions are needed, (i) the number of LCI result per group of number of dimensions decreases (Figure S 6), and (ii) the elementary flow values are lower (Figure S 7). For the first observation (i), the difference in information per elementary flows between groups that need 50 or 51 dimensions is low compared to the groups that only need 1 or 2 dimensions. The number of LCI result per group covers the high numbers of dimensions.

The second observation (ii) implies that when the information covers a high number of dimensions, elementary flow values tend to $1/\sqrt{n}$ (where n is the number of dimensions). Some LCI results still present a strong heterogeneity with a very high first elementary flow (although less than 0.95) with lower extra elementary flows that are needed for 0.95 to be reached, as demonstrated in Figure S 7 where high extreme values of elementary flows are observed when a high number of dimensions is needed.

Concerning the impact categories, the CF values express the modelled dangerousness of elementary flows towards environmental concerns. Expressed in kg of environmental indicator equivalents per kg (or Bq or J) of elementary flow, the standardization is applied by multiplying the CFs by the geometric means of the cumulated LCI database (expressed in kg or Bq or J of elementary flow). Considering one impact category, all its standardized CFs have the same unit: indicator equivalent.

This standardization brings forth the key dimensions where the LCI results of the cumulated LCI database have a globally high contribution on each impact category: it is the LCA results of the average LCI result of the database.

Standardized impact categories reveal the critical dimensions that are characterized by the modelled environmental issues as well as the dimensions that highly contribute to the impact categories by taking into account the global trend observed over the cumulated LCI database. The standardized impact category vectors are given in Annex B - 7.

Annex B-3: RI results according to standardized elementary flows and CFs

The RI of a LCI result for an impact category is the cosine of the angle between a standardized LCI result vector and a standardized impact category vector. The representativeness of an impact category regarding a LCI result relies on the direction of the two vectors, which depends on the similarity between the standardized elementary flows and the standardized CFs. An impact category is representative of a LCI result if the dimensions for which the LCI result distinguished itself from the cumulated LCI database are those for which the database produces a high global impact (cf. Annex B - 1). From a database point of view, high RIs reveal LCI results that strongly emit for dimensions that are globally high contributors towards the concerned impact categories.
In other words, when a LCI result emits above the average of the database for one or several dimensions and when the standardized CFs of these dimensions are also very high for an impact category, it should be sufficiently relevant to study this LCI result through this category with regard to all modelled product.
Considering the global trend of the cumulated LCI database, emissions of the LCI result are high for one or several dimensions that are also, globally, the strongest contributors to the impact category.
The RI values (from all LCI results of ecoinvent for one impact category) plotted as a function of the elementary flow that is the first contributor of the RI, suggests these values are correlated, as illustrated in Figure S 8 for climate change. The major trend of the RI is driven by its first contributor. Considering these particular first elementary flows and their related CFs, the values of their multiplications have also been plotted (black dots): this represents the part of the RI that is provided by the first contributor.

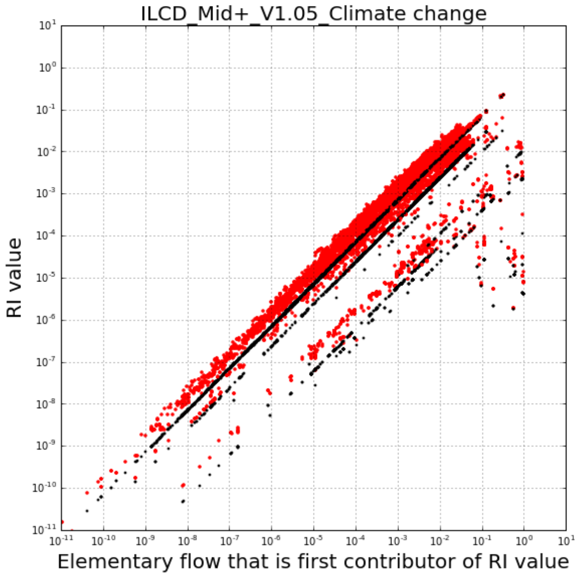


Figure S 8. RI values as a function of their first elementary flow contributors (red dots) and parts of the RI provided by the first contributor (black dots).

The Figure S 8 illustrates that only a few dimensions support the first elementary flows for this impact category. This small number of dimensions, represented by straight black lines, is essentially determined by the higher CFs of the impact category. Very few first elementary flows are found between 0.1 and 1. Yet, we previously observed that most of the first standardized elementary flows of LCI results are within this interval.

For the majority of LCI results, the first contributor of the RIs does not lie within the first ranked elementary flows but within the first ranked CFs.

Figure S 9 is a plot of RI values with the rank of the first elementary flow contributor per LCI result. It suggests that this first contributor is capable of having a very high rank and not lie amongst the very first elementary flows that support its norm.

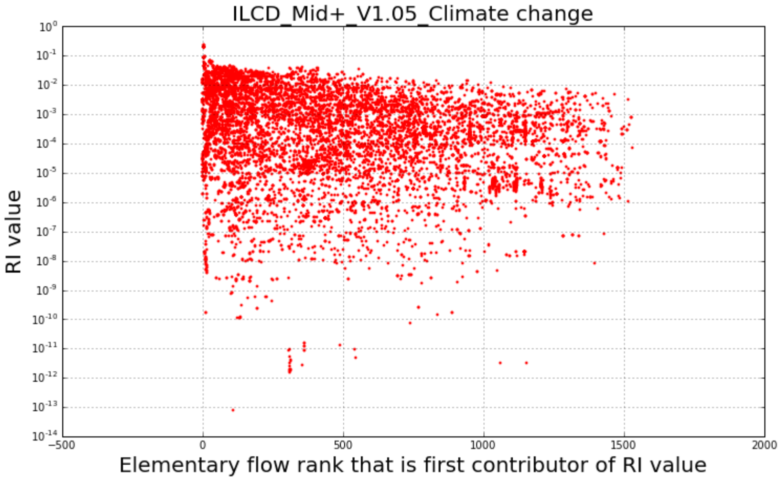


Figure S 9. RI values as a function of the rank of the first elementary flow contributor

RIs between 10^{-4} and 10^{-6} that are related to very high first elementary flows (1 to 0.1) highlight dimensions that have low CFs. Only very few LCI results use these dimensions as first elementary flows contributing to their RI. The value of the RI is provided by the best compromise between high CFs and high elementary flows. However, values of high CFs that endorse the global impact of the database on the environmental issue, most often bear more weight on the RI values. RIs provide an interesting insight on the intensity of the elementary flow of each of the studied LCI results over the critical dimensions determined for the impact category. For one LCI result, the impact category that has the highest RI is the impact category with best compromise between high elementary flow intensities and high CFs.

Moreover, the distance observed in Figure S 8 between the RI and the multiplication between the elementary flow and its CF that are the first contributors of the RI, reveals that the RI values are combinations of different dimensions. If no other dimensions contribute to the RI, the scatterplot would overlay the straight line.

Annex B-4: RI distributions per number of representative elementary flows per combination for each impact category of the ILCD

The following figures present the RI distributions of the LCI results of the whole database. For each impact category of the ILCD, LCI results are segregated by the number of elementary flows needed to obtain 95% of the value of the RI.

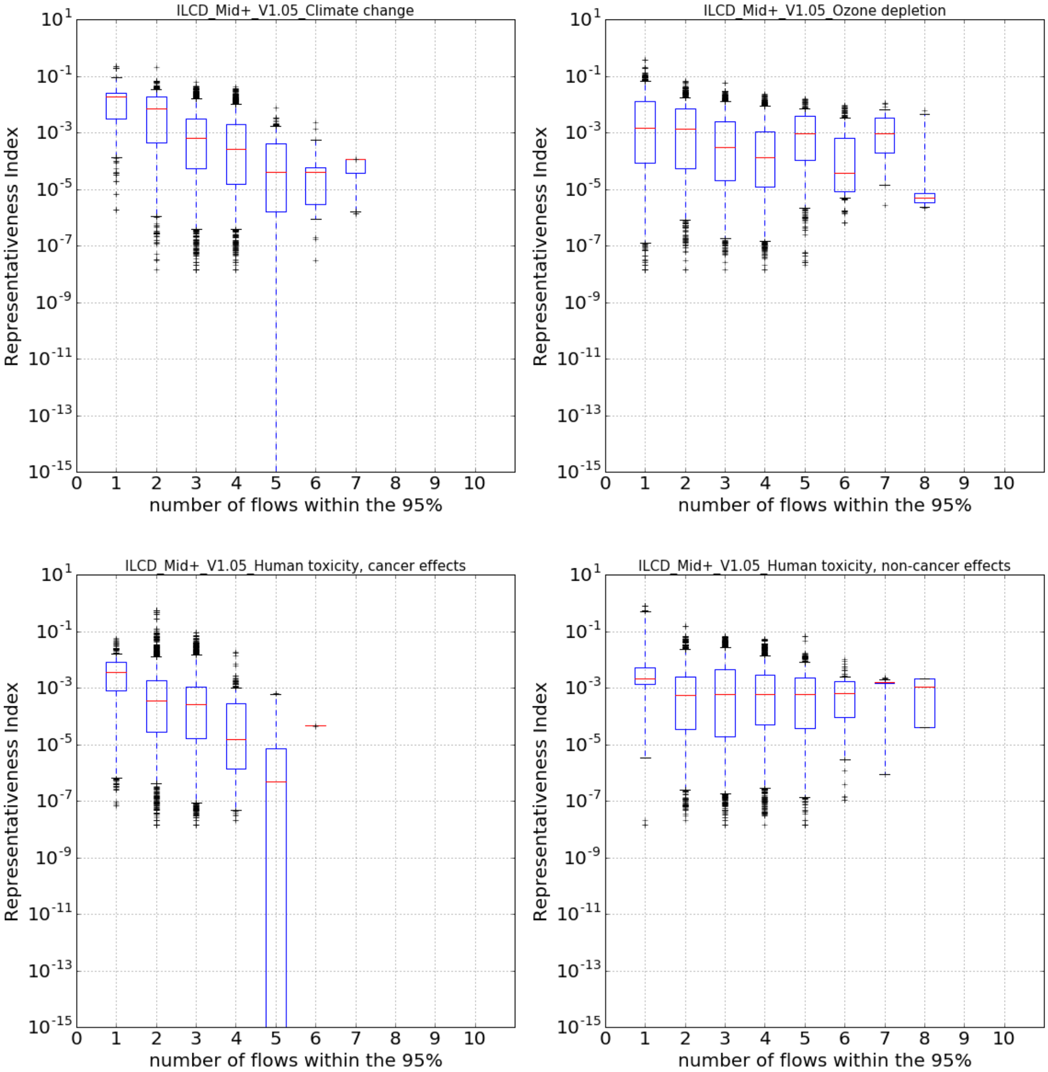


Figure S 10. RI distributions for Climate Change, Ozone depletion, Human toxicities cancer and non-cancer effects

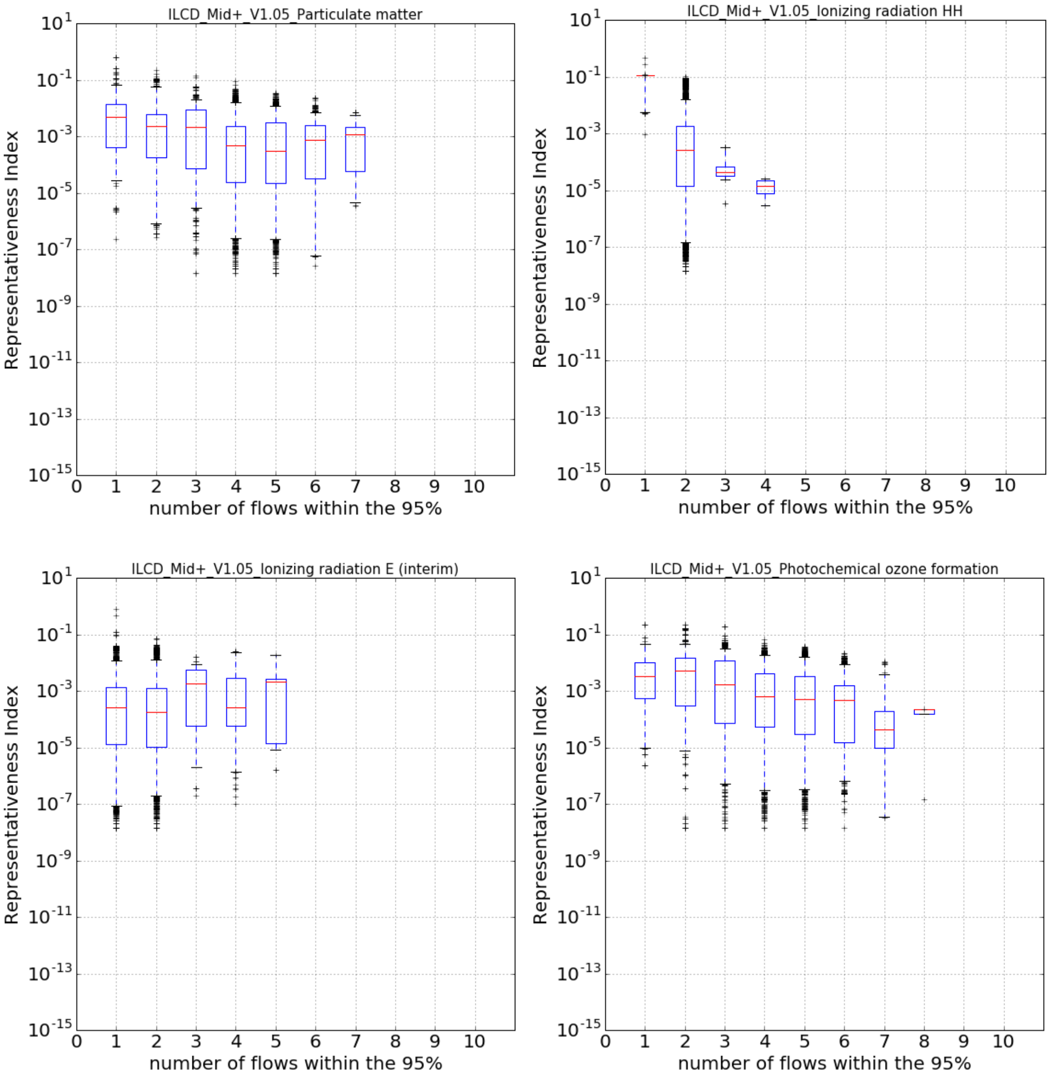


Figure S 11. RI distributions for Particulate matter, Ionizing radiations (HH and E) and Photochemical ozone formation

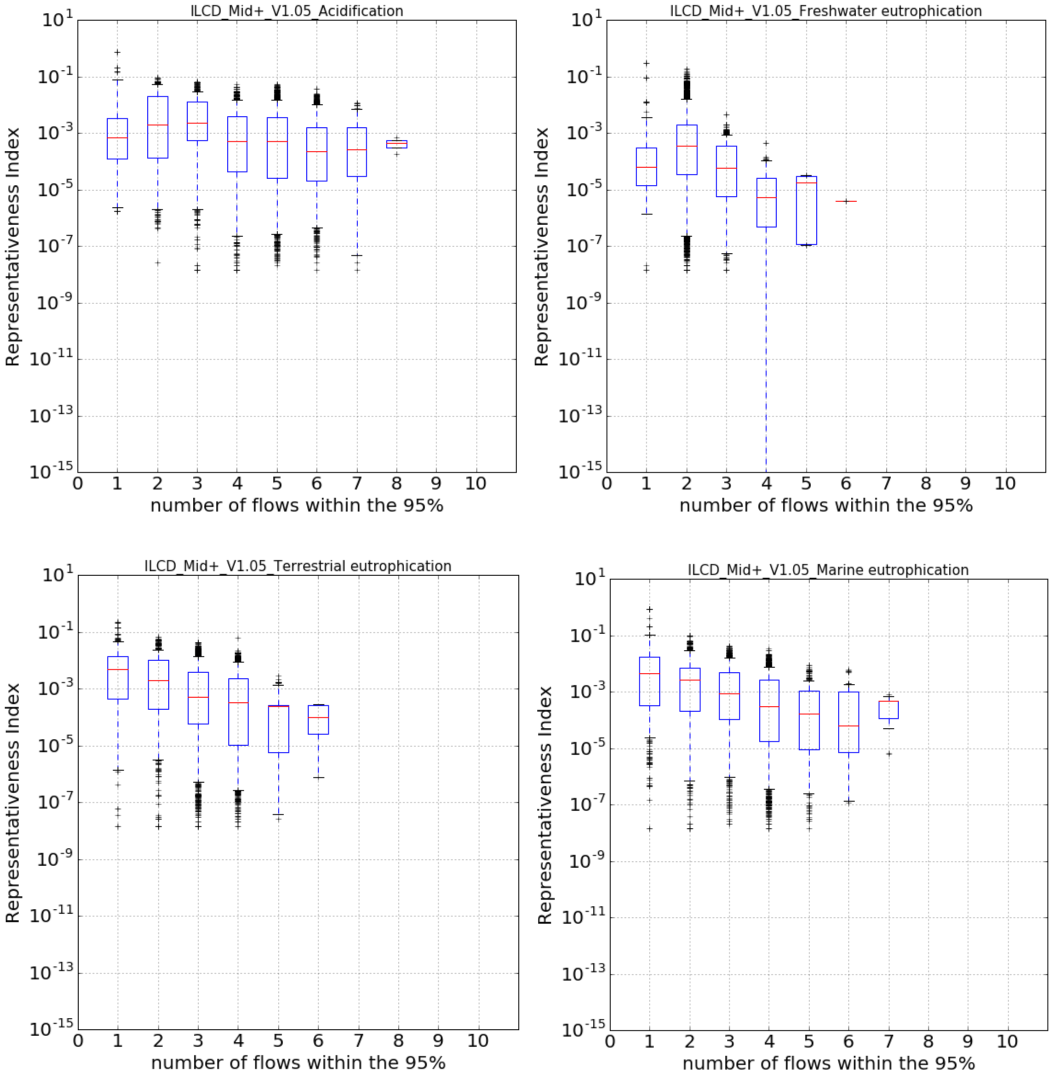


Figure S 12. RI distributions for Acidification, freshwater, terrestrial and marine Eutrophications

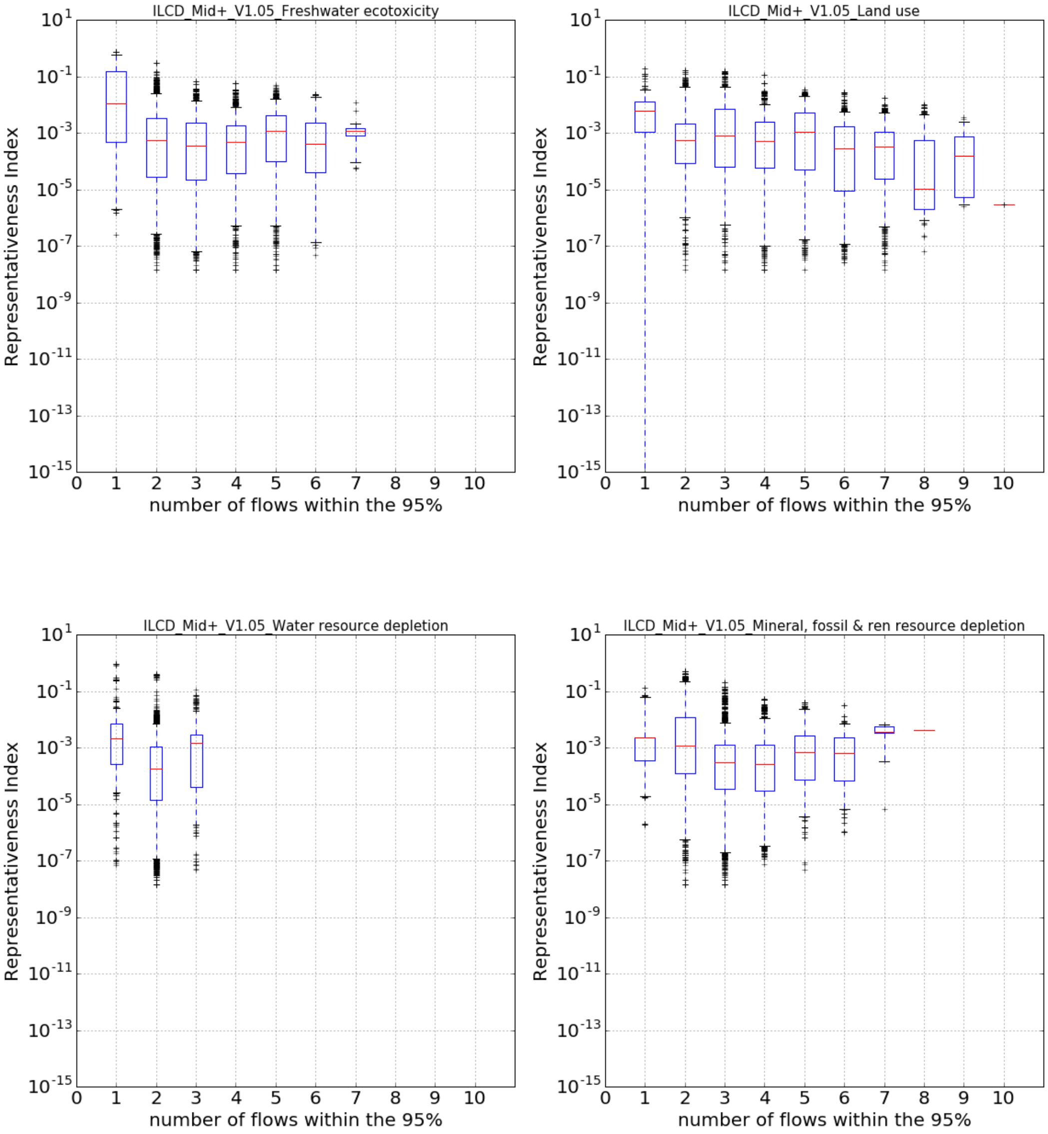


Figure S 13. RI distributions for Freshwater ecotoxicity, Land use, Resource depletion (water and mineral, fossil and renewable)

Annex B-5: Scatter matrix of the (RIortho – RIoriginal) / RIoriginal ratio per subset

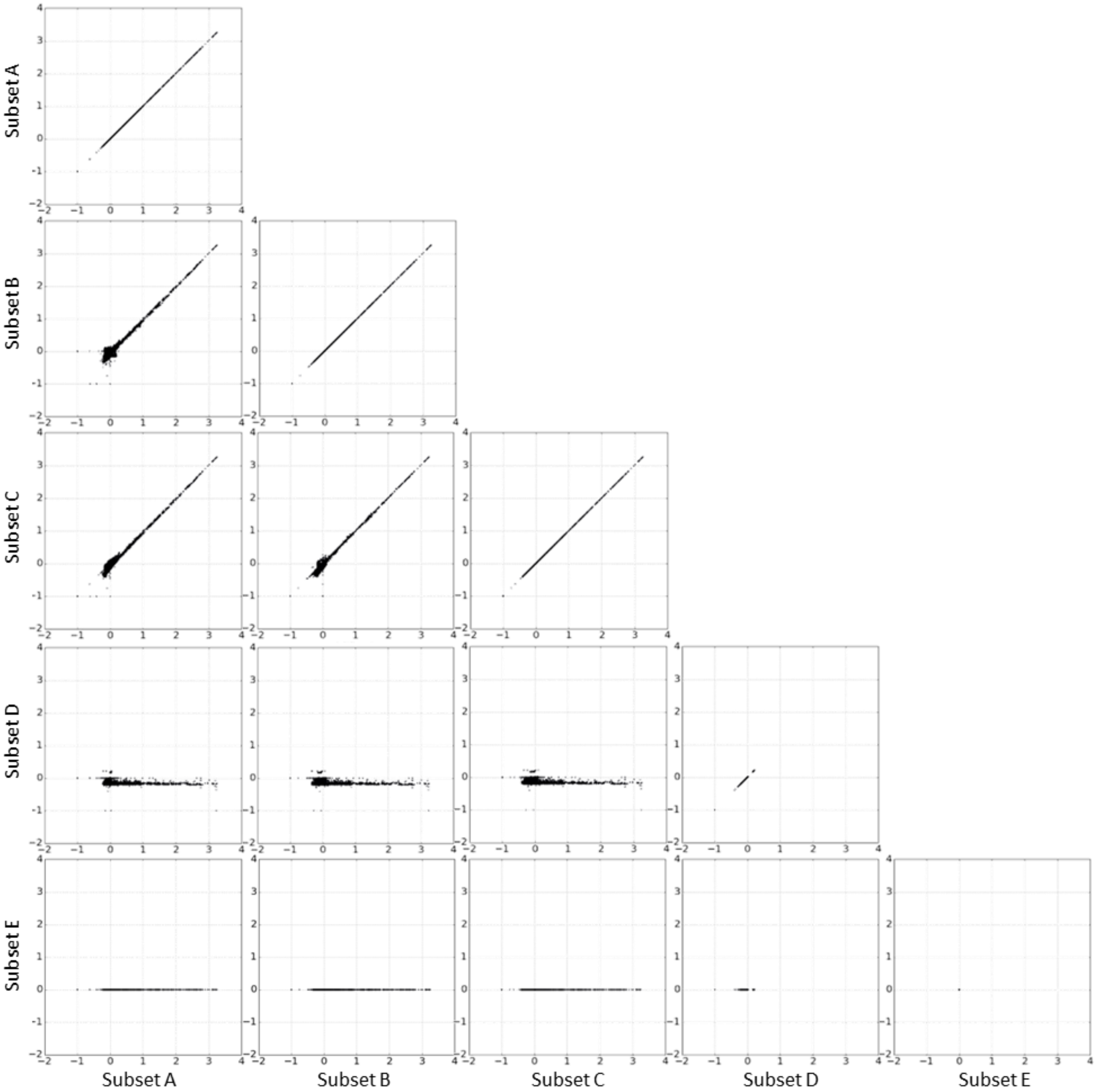


Figure S 14. Scatter matrix of the (RI_{ortho} – $RI_{original}$) / $RI_{original}$ ratio for the different impact categories per subset

Annex B-6: RI results obtained from the python toolbox

This excel file presents the result sheets obtained from the developed Python scritp. It is available from an online deposit with the DOI: 10.5281/zenodo.1068914. The package allows to apply the methodology on LCI excel files (system process) exported from SimaPro and modelled within the ecoinvent 3.1 database “allocation at the point of substitution” (further development have to be done to apply the methodology on other database and on LCI files exported from other software).

Three outputs can be obtained: global RIs of LCIA methods, RIs of their impact categories and RIs of the decorrelated RIs. Almost all the multi-criteria LCIA methods can be analysed. RIs of LCIA methodology and impact categories (orthogonalized or not) can be obtained.

Only RIs of the impact categories of the ILCD Mid+ V1.05 are presented.

Results are from the analyses of the Chinese and the German electricity mix production.

Table S 1. Global RIs of LCIA methods

LCIA method	Chinese electricity mix production	German electricity mix production
ILCD_Mid+_V1.05	1.13E-01	2.72E-02
ReCiPe_Mid_E_V1.11	9.02E-02	3.29E-02
ReCiPe_Mid_H_V1.11	9.19E-02	3.68E-02
ReCiPe_Mid_I_V1.11	1.03E-01	3.66E-02
ReCiPe_End_E_V1.11_Damage	3.92E-02	1.74E-02
ReCiPe_End_H_V1.11_Damage	5.93E-02	1.36E-02
ReCiPe_End_I_V1.11_Damage	7.15E-02	1.21E-02
ReCiPe_End_E_V1.11_End_	1.04E-01	3.31E-02
ReCiPe_End_H_V1.11_End_	1.06E-01	3.70E-02
ReCiPe_End_I_V1.11_End_	1.16E-01	3.69E-02
CML-IA_baseline_V3.02	8.88E-02	2.76E-02
TRACI_2.1_V1.02	8.25E-02	1.91E-02
Impact_2002+_V2.12	8.67E-02	3.11E-02
Eco_Scarc_2013_V1.01	8.68E-02	8.81E-02
EPD_2013_V1.01	7.63E-02	1.77E-02
EPS_2000_V2.08	1.22E-01	1.18E-02
EDIP_2003_V1.05	9.52E-02	5.94E-02
BEES_V4.05	1.01E-01	2.08E-02

Table S 2. RIs of the ILCD impact categories

ILCD, Impact category	Chinese electricity mix production	German electricity mix production
Climate change	3.54E-02	8.02E-03
Ozone depletion	1.99E-03	5.32E-03
Human toxicity, cancer effects	3.40E-03	4.22E-03
Human toxicity, non-cancer effects	7.35E-03	6.44E-03
Particulate matter	9.77E-02	1.24E-03
Ionizing radiation HH	5.50E-03	1.75E-02
Ionizing radiation E (interim)	1.84E-03	5.95E-03
Photochemical ozone formation	4.43E-02	2.68E-03
Acidification	6.42E-02	2.20E-03
Terrestrial eutrophication	3.79E-02	2.41E-03
Freshwater eutrophication	7.57E-03	1.57E-02
Marine eutrophication	1.74E-02	1.20E-03
Freshwater ecotoxicity	3.12E-03	4.48E-03
Land use	4.33E-03	1.24E-03
Water resource depletion	6.12E-17	1.49E-08
Mineral, fossil & ren resource depletion	5.84E-04	7.06E-04

Table S 3. Decorrelated RIs of the ILCD impact categories

ILCD, Impact category	Chinese electricity mix production	German electricity mix production
Climate change	3.53E-02	7.56E-03
Ozone depletion	1.99E-03	5.02E-03
Human toxicity, cancer effects	3.40E-03	3.97E-03
Human toxicity, non-cancer effects	7.34E-03	6.07E-03
Particulate matter	7.89E-02	8.19E-04
Ionizing radiation HH	5.43E-03	1.72E-02
Ionizing radiation E (interim)	1.82E-03	5.85E-03
Photochemical ozone formation	3.57E-02	1.53E-03
Acidification	5.19E-02	1.45E-03
Terrestrial eutrophication	3.06E-02	1.59E-03
Freshwater eutrophication	7.57E-03	1.57E-02
Marine eutrophication	1.41E-02	7.92E-04
Freshwater ecotoxicity	3.12E-03	4.22E-03
Land use	4.33E-03	1.24E-03
Water resource depletion	6.12E-17	1.49E-08
Mineral, fossil & ren resource depletion	5.84E-04	7.06E-04

Annex B-7: RI description per LCI through the main elementary flows

The following tables correspond to the analysis of the elementary flows that contribute the most to RIs of both of the studied LCI. The LCIA method used is the ILCD.
RIs are determined with the database under the ecoinvent elementary flow nomenclature and not with the simapro elementary flow nomenclature.

LCI: electricity, high voltage//[CN] market for electricity, high voltage
Global RI of the method: 1.13E-01

Table S 4. Elementary flows supporting impact category RIs for the Chinese electricity mix

Impact category	Elementary flows	Dimension contribution of the RI	Impact category RI	Std elementary flow value	Std elementary flow rank	Std CF value	Std CF rank
particulate matter	particulates, < 2.5 um to air urban air close to ground	7.65E-02	9.74E-02	8.60E-02	19	8.90E-01	0
	sulfur dioxide to air urban air close to ground	1.66E-02		8.15E-02	21	2.04E-01	3
acidification	sulfur dioxide to air urban air close to ground	4.32E-02	6.40E-02	8.15E-02	21	5.30E-01	1
	nitrogen oxides to air urban air close to ground	1.27E-02		5.96E-02	26	2.12E-01	3
	sulfur dioxide to air non-urban air or from high stacks	7.56E-03		9.98E-03	107	7.58E-01	0
photochemical ozone formation	nitrogen oxides to air urban air close to ground	3.55E-02	4.41E-02	5.96E-02	26	5.95E-01	1
	sulfur dioxide to air urban air close to ground	5.54E-03		8.15E-02	21	6.80E-02	6
terrestrial eutrophication	nitrogen oxides to air urban air close to ground	3.66E-02	3.78E-02	5.96E-02	26	6.14E-01	1
climate change	carbon dioxide, fossil to air urban air close to ground	2.53E-02	3.53E-02	3.66E-02	47	6.92E-01	0
	methane, fossil to air non-urban air or from high stacks	5.00E-03		5.22E-02	30	9.57E-02	3
	carbon dioxide, fossil to air non-urban air or from high stacks	4.07E-03		6.01E-03	141	6.77E-01	1

marine eutrophication	nitrogen oxides to air urban air close to ground	1.63E-02	1.74E-02	5.96E-02	26	2.73E-01	2
water resource depletion	water, river to natural resource in water	5.62E-03	9.46E-03	5.81E-03	144	9.67E-01	0
	water, well, in ground to natural resource in water	3.76E-03		1.47E-02	80	2.55E-01	1
freshwater eutrophication	phosphate to water ground-, long-term	6.58E-03	7.55E-03	6.73E-03	132	9.77E-01	0
	phosphate to water ground-	9.67E-04		4.49E-03	222	2.15E-01	1
human toxicity, non-cancer effects	zinc, ion to water ground-, long-term	1.93E-03	7.33E-03	2.27E-03	306	8.50E-01	0
	arsenic, ion to water ground-, long-term	1.93E-03		3.77E-03	243	5.13E-01	1
	mercury to air urban air close to ground	1.71E-03		6.74E-02	24	2.54E-02	8
	zinc to air urban air close to ground	7.76E-04		3.87E-02	45	2.00E-02	9
	lead to air urban air close to ground	3.91E-04		5.23E-02	29	7.46E-03	12
ionizing radiation hh	radon-222 to air low population density, long-term	4.41E-03	5.48E-03	5.38E-03	193	8.19E-01	0
	carbon-14 to air non-urban air or from high stacks	8.83E-04		1.54E-03	440	5.73E-01	1
land use	transformation, to industrial area to natural resource land	2.25E-03	4.33E-03	8.21E-03	115	2.74E-01	3
	transformation, from unspecified to natural resource land	2.02E-03		1.16E-02	97	-1.75E-01	4
	transformation, to dump site to natural resource land	1.89E-03		4.95E-02	38	3.82E-02	12
	occupation, dump site to natural resource land	9.10E-04		3.64E-02	48	2.50E-02	15
	transformation, to mineral extraction site to natural resource land	7.42E-04		1.04E-03	624	7.12E-01	0
human toxicity, cancer effects	chromium vi to water ground-, long-term	2.95E-03	3.39E-03	2.99E-03	271	9.87E-01	0

freshwater ecotoxicity	zinc, ion to water ground-, long-term	1.39E-03	3.11E-03	2.27E-03	306	6.12E-01	1
	copper, ion to water ground-, long-term	5.94E-04		7.68E-04	833	7.74E-01	0
	nickel, ion to water ground-, long-term	3.69E-04		4.46E-03	224	8.28E-02	4
	chromium vi to water ground-, long-term	2.74E-04		2.99E-03	271	9.16E-02	3
	vanadium, ion to water ground-, long-term	1.97E-04		2.15E-03	316	9.16E-02	2
ozone depletion	methane, bromotrifluoro-, halon 1301 to air non-urban air or from high stacks	9.28E-04	1.99E-03	9.49E-04	670	9.78E-01	0
	ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, cfc-114 to air non-urban air or from high stacks	8.58E-04		6.27E-03	138	1.37E-01	1
ionizing radiation e (interim)	carbon-14 to air non-urban air or from high stacks	1.54E-03	1.84E-03	1.54E-03	440	9.99E-01	0
	cesium-137 to water ocean	2.17E-04		4.51E-03	216	4.80E-02	1
mineral, fossil & ren resource depletion	nickel, 1.98% in silicates, 1.04% in crude ore, in ground to natural resource in ground	1.66E-04	5.82E-04	9.31E-04	672	1.78E-01	1
	indium, 0.005% in sulfide, in 0.003%, pb, zn, ag, cd, in ground to natural resource in ground	1.60E-04		1.65E-04	1705	9.75E-01	0
	uranium, in ground to natural resource in ground	8.63E-05		4.57E-03	211	1.89E-02	8
	coal, hard, unspecified, in ground to natural resource in ground	4.54E-05		4.68E-02	41	9.70E-04	36

LCI: electricity, high voltage//[DE] market for electricity, high voltage

Global RI of the method: 2.85E-02

Table S 5. Elementary flows supporting impact category RIs for the German electricity mix

Impact category	Elementary flow	Dimension contribution of the RI	Impact category RI	Std elementary flow value	Std elementary flow rank	Std CF value	Std CF rank
ionizing radiation hh	radon-222 to air low population density, long-term	1.46E-02	1.76E-02	1.78E-02	222	8.19E-01	0
	carbon-14 to air non-urban air or from high stacks	2.63E-03		4.60E-03	543	5.73E-01	1
freshwater eutrophication	phosphate to water ground-, long-term	1.41E-02	1.58E-02	1.45E-02	308	9.77E-01	0
	phosphate to water ground-	1.68E-03		7.79E-03	448	2.15E-01	1
climate change	carbon dioxide, fossil to air non-urban air or from high stacks	6.25E-03	8.09E-03	9.23E-03	404	6.77E-01	1
	carbon dioxide, fossil to air urban air close to ground	1.09E-03		1.58E-03	888	6.92E-01	0
	methane, fossil to air non-urban air or from high stacks	4.89E-04		5.10E-03	524	9.57E-02	3
water resource depletion	water, river to natural resource in water	5.21E-03	7.37E-03	5.39E-03	517	9.67E-01	0
	water, well, in ground to natural resource in water	2.14E-03		8.38E-03	424	2.55E-01	1
human toxicity, non-cancer effects	zinc, ion to water ground-, long-term	2.82E-03	6.49E-03	3.32E-03	610	8.50E-01	0
	arsenic, ion to water ground-, long-term	2.79E-03		5.44E-03	514	5.13E-01	1
	mercury to air non-urban air or from high stacks	3.97E-04		9.22E-03	405	4.31E-02	4
ionizing radiation e (interim)	carbon-14 to air non-urban air or from high stacks	4.59E-03	6.00E-03	4.60E-03	543	9.99E-01	0
	cesium-137 to water ocean	7.76E-04		1.62E-02	284	4.80E-02	1
	iodine-131 to air non-urban air	3.52E-04		3.89E-01	1	9.04E-04	9

	or from high stacks						
ozone depletion	ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, cfc-114 to air non-urban air or from high stacks	2.89E-03	5.37E-03	2.12E-02	157	1.37E-01	1
	methane, bromochlorodifluoro-, halon 1211 to air non-urban air or from high stacks	1.53E-03		1.16E-02	373	1.32E-01	2
	methane, bromotrifluoro-, halon 1301 to air non-urban air or from high stacks	5.59E-04		5.72E-04	1286	9.78E-01	0
freshwater ecotoxicity	zinc, ion to water ground-, long-term	2.03E-03	4.52E-03	3.32E-03	610	6.12E-01	1
	copper, ion to water ground-, long-term	7.73E-04		9.99E-04	1044	7.74E-01	0
	nickel, ion to water ground-, long-term	7.04E-04		8.50E-03	420	8.28E-02	4
	chromium vi to water ground-, long-term	3.58E-04		3.91E-03	576	9.16E-02	3
	vanadium, ion to water ground-, long-term	3.27E-04		3.57E-03	592	9.16E-02	2
human toxicity, cancer effects	chromium vi to water ground-, long-term	3.86E-03	4.25E-03	3.91E-03	576	9.87E-01	0
photochemical ozone formation	nitrogen oxides to air non-urban air or from high stacks	1.60E-03	2.70E-03	2.54E-03	730	6.28E-01	0
	nitrogen oxides to air urban air close to ground	3.84E-04		6.45E-04	1247	5.95E-01	1
	nmvoc, non-methane volatile organic compounds, unspecified origin to air non-urban air or from high stacks	2.19E-04		1.11E-03	1000	1.98E-01	3
	nitrogen oxides to air unspecified	1.77E-04		4.09E-04	1436	4.33E-01	2
	sulfur dioxide to air non-urban air or from high stacks	1.40E-04		1.44E-03	914	9.72E-02	4
marine	nitrate to water ground-, long-	1.30E-03	2.51E-03	1.45E-03	909	8.96E-01	0

eutrophication	term						
	nitrogen oxides to air non-urban air or from high stacks	7.33E-04		2.54E-03	730	2.88E-01	1
	nitrogen oxides to air urban air close to ground	1.76E-04		6.45E-04	1247	2.73E-01	2
	nitrate to water ground-	1.38E-04		1.23E-02	345	1.12E-02	4
terrestrial eutrophication	nitrogen oxides to air non-urban air or from high stacks	1.65E-03	2.43E-03	2.54E-03	730	6.48E-01	0
	nitrogen oxides to air urban air close to ground	3.96E-04		6.45E-04	1247	6.14E-01	1
	nitrogen oxides to air unspecified	1.83E-04		4.09E-04	1436	4.47E-01	2
	ammonia to air non-urban air or from high stacks	1.31E-04		9.12E-03	406	1.44E-02	5
acidification	sulfur dioxide to air non-urban air or from high stacks	1.09E-03	2.21E-03	1.44E-03	914	7.58E-01	0
	nitrogen oxides to air non-urban air or from high stacks	5.70E-04		2.54E-03	730	2.24E-01	2
	sulfur dioxide to air urban air close to ground	1.86E-04		3.51E-04	1485	5.30E-01	1
	nitrogen oxides to air urban air close to ground	1.37E-04		6.45E-04	1247	2.12E-01	3
land use	transformation, from annual crop to natural resource land	9.29E-03	2.13E-03	3.08E-02	120	-3.02E-01	2
	transformation, to annual crop, non-irrigated, intensive to natural resource land	9.25E-03		1.87E-02	187	4.95E-01	1
	transformation, to annual crop, non-irrigated, extensive to natural resource land	5.85E-03		6.85E-02	24	8.55E-02	6
	transformation, from annual crop, non-irrigated, extensive to natural resource land	5.84E-03		6.92E-02	22	-8.43E-02	7
	transformation, to annual crop to natural resource land	3.44E-03		4.38E-02	55	7.86E-02	8
	transformation, from annual crop, non-irrigated, intensive	2.45E-03		2.20E-02	154	-1.11E-01	5

	to natural resource land						
particulate matter	sulfur dioxide to air non-urban air or from high stacks	3.84E-04	1.25E-03	1.44E-03	914	2.68E-01	2
	particulates, < 2.5 um to air urban air close to ground	3.09E-04		3.48E-04	1491	8.90E-01	0
	particulates, < 2.5 um to air non-urban air or from high stacks	2.46E-04		9.06E-04	1056	2.72E-01	1
	particulates, < 2.5 um to air unspecified	8.31E-05		6.40E-04	1249	1.30E-01	4
	sulfur dioxide to air urban air close to ground	7.17E-05		3.51E-04	1485	2.04E-01	3
mineral, fossil & ren resource depletion	uranium, in ground to natural resource in ground	2.85E-04	7.12E-04	1.51E-02	299	1.89E-02	8
	indium, 0.005% in sulfide, in 0.003%, pb, zn, ag, cd, in ground to natural resource in ground	1.91E-04		1.96E-04	1718	9.75E-01	0
	nickel, 1.98% in silicates, 1.04% in crude ore, in ground to natural resource in ground	8.45E-05		4.74E-04	1379	1.78E-01	1

Annex B-8: Main standardized Characterization Factors per impact category of the ILCD

The following tables correspond to the main CFs for each impact category of the ILCD obtained after the standardization procedure. Only the first eight CFs per impact category are presented due to the high number of CFs.

Table S 6. Main CFs of Climate Change

Dimension	Climate change
carbon dioxide, fossil to air urban air close to ground	6.92E-01
carbon dioxide, fossil to air non-urban air or from high stacks	6.77E-01
carbon dioxide, fossil to air unspecified	2.32E-01
methane, fossil to air non-urban air or from high stacks	9.57E-02
dinitrogen monoxide to air urban air close to ground	1.09E-02
methane, fossil to air urban air close to ground	8.05E-03
methane, fossil to air unspecified	7.05E-03
dinitrogen monoxide to air non-urban air or from high stacks	5.88E-03

Table S 7. Main CFs of Ozone depletion

Dimension	Ozone depletion
methane, bromotrifluoro-, halon 1301 to air non-urban air or from high stacks	9.78E-01
ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, cfc-114 to air non-urban air or from high stacks	1.37E-01
methane, bromochlorodifluoro-, halon 1211 to air non-urban air or from high stacks	1.32E-01
methane, tetrachloro-, r-10 to air urban air close to ground	5.57E-02
methane, dichlorodifluoro-, cfc-12 to air urban air close to ground	5.39E-02
ethane, 1,1,2-trichloro-1,2,2-trifluoro-, cfc-113 to air unspecified	2.86E-02
methane, chlorodifluoro-, hcfc-22 to air non-urban air or from high stacks	2.46E-02
methane, chlorodifluoro-, hcfc-22 to air urban air close to ground	1.70E-02

Table S 8. Main CFs of Human toxicity, cancer effects

Dimension	Human toxicity, cancer effects
chromium vi to water ground-, long-term	9.87E-01
chromium vi to water surface water	1.51E-01
chromium to air non-urban air or from high stacks	3.58E-02
nickel, ion to water ground-, long-term	2.27E-02
arsenic, ion to water ground-, long-term	1.77E-02
chromium, ion to water surface water	4.55E-03
chromium, ion to water unspecified	3.88E-03
chromium vi to soil unspecified	3.56E-03

Table S 9. Main CFs of Human toxicity, non-cancer effects

Dimension	Human toxicity, non-cancer effects
zinc, ion to water ground-, long-term	8.50E-01
arsenic, ion to water ground-, long-term	5.13E-01
mercury to air unspecified	6.20E-02
zinc to air non-urban air or from high stacks	5.99E-02
mercury to air non-urban air or from high stacks	4.31E-02
arsenic, ion to water surface water	3.25E-02
lead to air non-urban air or from high stacks	3.03E-02
zinc to air unspecified	2.96E-02

Table S 10. Main CFs of Particulate matter

Dimension	Particulate matter
particulates, < 2.5 um to air urban air close to ground	8.90E-01
particulates, < 2.5 um to air non-urban air or from high stacks	2.72E-01
sulfur dioxide to air non-urban air or from high stacks	2.68E-01
sulfur dioxide to air urban air close to ground	2.04E-01
particulates, < 2.5 um to air unspecified	1.30E-01
sulfur dioxide to air unspecified	5.58E-02
nitrogen oxides to air urban air close to ground	1.69E-02
nitrogen oxides to air non-urban air or from high stacks	1.66E-02

Table S 11. Main CFs of Ionizing radiation HH

Dimension	Ionizing radiation HH
radon-222 to air low population density, long-term	8.19E-01
carbon-14 to air non-urban air or from high stacks	5.73E-01
radon-222 to air non-urban air or from high stacks	2.33E-02
cesium-137 to water surface water	1.07E-03
cobalt-60 to water surface water	7.42E-04
uranium-234 to air non-urban air or from high stacks	6.04E-04
iodine-129 to air non-urban air or from high stacks	4.60E-04
radium-226 to water surface water	3.76E-04

Table S 12. Main CFs of Ionizing radiation E (interim)

Dimension	Ionizing radiation E (interim)
carbon-14 to air non-urban air or from high stacks	9.99E-01
cesium-137 to water ocean	4.80E-02
hydrogen-3, tritium to water surface water	1.48E-02
hydrogen-3, tritium to water ocean	1.12E-02
antimony-124 to water surface water	8.08E-03
cobalt-60 to water surface water	4.78E-03
cesium-137 to water surface water	3.39E-03
cobalt-58 to water surface water	3.27E-03

Table S 13. Main CFs of Photochemical ozone formation

Dimension	Photochemical ozone formation
nitrogen oxides to air non-urban air or from high stacks	6.28E-01
nitrogen oxides to air urban air close to ground	5.95E-01
nitrogen oxides to air unspecified	4.33E-01
nmvoc, non-methane volatile organic compounds, unspecified origin to air non-urban air or from high stacks	1.98E-01
sulfur dioxide to air non-urban air or from high stacks	9.72E-02
nmvoc, non-methane volatile organic compounds, unspecified origin to air unspecified	7.66E-02
sulfur dioxide to air urban air close to ground	6.80E-02
nmvoc, non-methane volatile organic compounds, unspecified origin to air urban air close to ground	6.48E-02

Table S 14. Main CFs of Acidification

Dimension	Acidification
sulfur dioxide to air non-urban air or from high stacks	7.58E-01
sulfur dioxide to air urban air close to ground	5.30E-01
nitrogen oxides to air non-urban air or from high stacks	2.24E-01
nitrogen oxides to air urban air close to ground	2.12E-01
sulfur dioxide to air unspecified	1.58E-01
nitrogen oxides to air unspecified	1.55E-01
ammonia to air unspecified	2.43E-02
ammonia to air urban air close to ground	9.99E-03

Table S 15. Main CFs of Terrestrial eutrophication

Dimension	Terrestrial eutrophication
nitrogen oxides to air non-urban air or from high stacks	6.48E-01
nitrogen oxides to air urban air close to ground	6.14E-01
nitrogen oxides to air unspecified	4.47E-01
ammonia to air unspecified	5.45E-02
ammonia to air urban air close to ground	2.24E-02
ammonia to air non-urban air or from high stacks	1.44E-02
nitrogen oxides to air lower stratosphere + upper troposphere	1.78E-05
nitrate to air unspecified	1.14E-05

Table S 16. Main CFs of Freshwater eutrophication

Dimension	**Freshwater eutrophication**
phosphate to water ground-, long-term	9.77E-01
phosphate to water ground-	2.15E-01
phosphate to water surface water	2.10E-03
phosphorus to water surface water	1.98E-03
phosphorus to soil agricultural	1.33E-03
phosphorus to soil industrial	4.23E-04
phosphate to water ocean	1.45E-04
phosphorus to water ocean	3.73E-05

Table S 17. Main CFs of Marine eutrophication

Dimension	**Marine eutrophication**
nitrate to water ground-, long-term	8.96E-01
nitrogen oxides to air non-urban air or from high stacks	2.88E-01
nitrogen oxides to air urban air close to ground	2.73E-01
nitrogen oxides to air unspecified	1.99E-01
nitrate to water ground-	1.12E-02
nitrate to water surface water	9.37E-03
ammonium, ion to water ground-, long-term	7.18E-03
ammonium, ion to water surface water	6.71E-03

Table S 18. Main CFs of Freshwater ecotoxicity

Dimension	Freshwater ecotoxicity
copper, ion to water ground-, long-term	7.74E-01
zinc, ion to water ground-, long-term	6.12E-01
vanadium, ion to water ground-, long-term	9.16E-02
chromium vi to water ground-, long-term	9.16E-02
nickel, ion to water ground-, long-term	8.28E-02
antimony to water ground-, long-term	3.67E-02
arsenic, ion to water ground-, long-term	1.81E-02
chromium vi to water surface water	1.40E-02

Table S 19. Main CFs of Land use

Dimension	Land use
transformation, to mineral extraction site to natural resource land	7.12E-01
transformation, to annual crop, non-irrigated, intensive to natural resource land	4.95E-01
transformation, to industrial area to natural resource land	2.74E-01
transformation, to annual crop, non-irrigated, extensive to natural resource land	8.55E-02
transformation, to annual crop to natural resource land	7.86E-02
occupation, forest, intensive to natural resource land	7.45E-02
transformation, to dump site to natural resource land	3.82E-02
transformation, to traffic area, road network to natural resource land	3.72E-02

Table S 20. Main CFs of Water resource depletion

Dimension	Water resource depletion
water, river to natural resource in water	9.67E-01
water, well, in ground to natural resource in water	2.55E-01
water, lake to natural resource in water	8.34E-03

Table S 21. Main CFs of Mineral, fossil and renewable resource depletion

Dimension	Mineral, fossil & ren resource depletion
indium, 0.005% in sulfide, in 0.003%, pb, zn, ag, cd, in ground to natural resource in ground	9.75E-01
nickel, 1.98% in silicates, 1.04% in crude ore, in ground to natural resource in ground	1.78E-01
cadmium, 0.30% in sulfide, cd 0.18%, pb, zn, ag, in, in ground to natural resource in ground	1.17E-01
silver, ag 9.7e-4%, in mixed ore, in ground to natural resource in ground	3.11E-02
copper, 0.99% in sulfide, cu 0.36% and mo 8.2e-3% in crude ore, in ground to natural resource in ground	2.74E-02
lead, 5.0% in sulfide, pb 3.0%, zn, ag, cd, in, in ground to natural resource in ground	2.67E-02
silver, 0.007% in sulfide, ag 0.004%, pb, zn, cd, in, in ground to natural resource in ground	2.16E-02
tantalum, 81.9% in tantalite, 1.6e-4% in crude ore, in ground to natural resource in ground	2.14E-02

Annex B-9: Occurrence of representative elementary flows

For each impact categories, the following tables reference the main representative elementary flows based on an occurrence analysis. These elementary flows are the ones that most often provide 95% of the RI values for each LCI. The columns correspond to the number of different elementary flows per combination. Table are limited to the first eight main elementary flows.

For example in Table S 22, there are 4194 different LCIs which have the elementary flow “carbon dioxide, fossil to air non-urban air or from high stacks” that appear in the combination of three elementary flows that are needed to get up to 95% of the value of their Climate Change RIs. This elementary flow is also the one that is the most frequent within all RIs: it is present within 28% of all combinations.

Table S 22. Occurrences of the main elementary flows in RIs of Climate Change

Elementary flow	1	2	3	4	5	6	7	total	% of total occurrence
carbon dioxide, fossil to air non-urban air or from high stacks	329	783	4194	4619	556	42	123	10646	28%
carbon dioxide, fossil to air urban air close to ground	203	812	4209	4630	556	42	123	10575	56%
carbon dioxide, fossil to air unspecified	18	61	2962	4327	504	42	123	8037	77%
methane, fossil to air non-urban air or from high stacks	2	124	799	3503	223	5		4656	90%
dinitrogen monoxide to air urban air close to ground		12	75	458	222	21	50	838	92%
dinitrogen monoxide to air non-urban air or from high stacks		24	125	279	233	34	123	818	94%
methane, fossil to air urban air close to ground		141	278	178	28	1		626	96%
methane, non-fossil to air non-urban air or from high stacks	8	11	25	168	177	12	112	513	97%

Table S 23. Occurrences of the main elementary flows in RIs of Ozone Depletion

Elementary flow	1	2	3	4	5	6	7	8	total	% of total occurrence
methane, bromotrifluoro-, halon 1301 to air non-urban air or from high stacks	1681	2095	2593	2199	1275	772	66	19	10700	31%
ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, cfc-114 to air non-urban air or from high stacks	128	653	1944	2088	961	760	65	19	6618	50%
methane, bromochlorodifluoro-, halon 1211 to air non-urban air or from high stacks	118	533	2070	2074	929	738	66	19	6547	69%
methane, tetrachloro-, r-10 to air urban air close to ground	45	532	529	1090	916	605	62	19	3798	80%
methane, dichlorodifluoro-, cfc-12 to air urban air close to ground	26	156	411	754	978	770	66	19	3180	89%
methane, chlorodifluoro-, hcfc-22 to air non-urban air or from high stacks		170	114	370	439	291	27	19	1430	93%
methane, chlorodifluoro-, hcfc-22 to air urban air close to ground	2	2	131	62	419	476	62	19	1173	96%
ethane, 1,1,2-trichloro-1,2,2-trifluoro-, cfc-113 to air unspecified	41	208	67	131	192	206	43	19	907	99%

Table S 24. Occurrences of the main elementary flows in RIs of Human toxicity, cancer effects

Elementary flow	1	2	3	4	5	6	total	% of total occurrence
chromium vi to water ground-, long-term	808	5005	4502	837	34	3	11189	40%
chromium vi to water surface water	3	4384	4364	834	33	3	9621	75%
chromium to air non-urban air or from high stacks	2		2839	471	27	3	3342	87%
arsenic, ion to water ground-, long-term		374	307	209	6		896	90%
chromium, ion to water surface water		10	438	298	22		768	93%
chromium, ion to water ground-		27	192	247	22		488	94%
chromium, ion to water unspecified		38	253	61			352	96%
chromium vi to soil unspecified		86	154	57	1		298	97%

Table S 25. Occurrences of the main elementary flows in RIs of Human toxicity, non-cancer effects

Elementary flow	1	2	3	4	5	6	7	8	total	% of total occurrence
zinc, ion to water ground-, long-term	107	2220	3932	2933	1397	247	92	4	10932	29%
arsenic, ion to water ground-, long-term		2126	3796	2767	1376	243	89	4	10401	57%
mercury to air unspecified		2	640	1703	802	86	15	4	3252	65%
zinc to air non-urban air or from high stacks		3	367	954	389	81	7		1801	70%
mercury to air non-urban air or from high stacks		7	914	318	366	98	75	2	1780	75%
zinc to air unspecified	7	3	82	777	495	45	12		1421	79%
mercury to air urban air close to ground	4	36	577	304	171	124	67	2	1285	82%
arsenic, ion to water surface water	26	29	289	442	234	68	2	4	1094	85%

Table S 26. Occurrences of the main elementary flows in RIs of Particulate matter

Elementary flow	1	2	3	4	5	6	7	total	% of total occurrence
particulates, < 2.5 um to air urban air close to ground	286	671	818	3701	4074	1104	117	10771	23%
sulfur dioxide to air non-urban air or from high stacks	42	231	559	3592	4069	1096	117	9706	43%
particulates, < 2.5 um to air non-urban air or from high stacks	44	155	495	3498	4007	1099	117	9415	63%
sulfur dioxide to air urban air close to ground	2	353	281	2903	3861	1088	117	8605	81%
particulates, < 2.5 um to air unspecified	18	100	152	556	3205	1069	117	5217	92%
sulfur dioxide to air unspecified	12	99	108	249	572	454	104	1598	95%
ammonia to air non-urban air or from high stacks		36	105	64	295	85	3	588	97%
nitrogen oxides to air non-urban air or from high stacks	3		52	50	85	211	22	423	97%

Table S 27. Occurrences of the main elementary flows in RIs of Ionizing radiation HH

Elementary flow	1	2	3	4	total	% of total occurrence
radon-222 to air low population density, long-term	98	11029	45	10	11182	50%
carbon-14 to air non-urban air or from high stacks	19	11029	45	10	11103	100%
uranium-234 to air non-urban air or from high stacks			30	10	40	100%
radon-222 to air non-urban air or from high stacks	3	2	6		11	100%
thorium-230 to air non-urban air or from high stacks				8	8	100%
polonium-210 to air urban air close to ground			5		5	100%
uranium-238 to water surface water			4		4	100%
radium-226 to water ocean				2	2	100%

Table S 28. Occurrences of the main elementary flows in RIs of Ionizing radiation E (interim)

Elementary flow	1	2	3	4	5	total	% of total occurrence
carbon-14 to air non-urban air or from high stacks	5155	5687	65	270	29	11206	62%
cesium-137 to water ocean		5686	65	270	29	6050	96%
hydrogen-3, tritium to water surface water		1	44	270	29	344	98%
antimony-124 to water surface water				270	29	299	100%
carbon-14 to water surface water					29	29	100%
iodine-131 to air non-urban air or from high stacks			21			21	100%

Table S 29. Occurrences of the main elementary flows in RIs of Photochemical ozone formation

Elementary flow	1	2	3	4	5	6	7	8	total	% of total occurrence
nitrogen oxides to air non-urban air or from high stacks	28	364	1364	3679	3556	1334	152	4	10481	22%
nitrogen oxides to air urban air close to ground	82	315	792	3439	3549	1332	131	4	9644	42%
nitrogen oxides to air unspecified	6	275	947	3142	3395	1323	151	4	9243	61%
nmvoc, non-methane volatile organic compounds, unspecified origin to air non-urban air or from high stacks	15	114	647	2102	2744	1157	137	4	6920	76%
sulfur dioxide to air non-urban air or from high stacks	6	145	222	766	1166	686	40		3031	82%
nmvoc, non-methane volatile organic compounds, unspecified origin to air unspecified	8	165	196	529	1262	581	53		2794	88%
nmvoc, non-methane volatile organic compounds, unspecified origin to air urban air close to ground		106	290	376	979	776	123	4	2654	93%
sulfur dioxide to air urban air close to ground		28	112	440	616	374	20		1590	97%

Table S 30. Occurrences of the main elementary flows in RIs of Acidification

Elementary flow	1	2	3	4	5	6	7	8	total	% of total occurrence
sulfur dioxide to air non-urban air or from high stacks	65	430	1525	2066	3426	2811	277	2	10602	21%
sulfur dioxide to air urban air close to ground	13	261	1267	1959	3417	2811	277	2	10007	40%
nitrogen oxides to air non-urban air or from high stacks	5	377	520	1384	2945	2760	277	2	8270	57%
nitrogen oxides to air urban air close to ground	41	242	768	961	2735	2734	277	2	7760	72%
sulfur dioxide to air unspecified	2	24	299	520	2810	2690	270	2	6617	85%
nitrogen oxides to air unspecified	1	48	349	944	1319	2377	273	2	5313	95%
ammonia to air non-urban air or from high stacks	78	88	61	233	149	228	58	2	897	97%
ammonia to air urban air close to ground		62	67	80	138	268	95	2	712	99%

Table S 31. Occurrences of the main elementary flows in RIs of Terrestrial eutrophication

Elementary flow	1	2	3	4	5	6	total	% of total occurrence
nitrogen oxides to air non-urban air or from high stacks	344	1039	5034	3786	287	10	10500	30%
nitrogen oxides to air urban air close to ground	198	685	4920	3787	288	10	9888	58%
nitrogen oxides to air unspecified	74	553	4819	3722	288	10	9466	85%
ammonia to air unspecified	24	97	120	2435	95	10	2781	93%
ammonia to air urban air close to ground		83	155	1045	271	10	1564	97%
ammonia to air non-urban air or from high stacks	50	256	161	373	211	10	1061	100%
nitrogen oxides to air lower stratosphere + upper troposphere			10				10	100%
nitrate to air unspecified		1	1				2	100%

Table S 32. Occurrences of the main elementary flows in RIs of Freshwater eutrophication

Elementary flow	1	2	3	4	5	6	total	% of total occurrence
phosphate to water ground-, long-term	253	9352	971	573	31	8	11188	46%
phosphate to water ground-		9167	928	571	31	8	10705	90%
phosphorus to water surface water		61	339	564	31	8	1003	94%
phosphate to water surface water	5	67	220	507	20	8	827	97%
phosphorus to soil agricultural	7	51	349	67	11	8	493	99%
phosphorus to water ground-		1	30	3	31	8	73	100%
phosphate to water ocean	2		42	5			49	100%
phosphorus to soil industrial	3	1	30				34	100%

Table S 33. Occurrences of the main elementary flows in RIs of Marine eutrophication

Elementary flow	1	2	3	4	5	6	7	total	% of total occurrence
nitrate to water ground-, long-term	575	1317	2126	5315	744	243	35	10355	27%
nitrogen oxides to air non-urban air or from high stacks	81	662	1854	5199	728	243	35	8802	51%
nitrogen oxides to air urban air close to ground	139	493	1473	5238	739	236	35	8353	73%
nitrogen oxides to air unspecified	58	273	768	5000	635	242	35	7011	92%
nitrate to water ground-	113	221	253	201	162	51	14	1015	94%
ammonium, ion to water surface water	11	69	89	110	248	206	35	768	96%
nitrate to water surface water	1	50	133	138	196	189	35	742	98%
ammonium, ion to water ground-, long-term	18	58	59	28	80	1	21	265	99%

Table S 34. Occurrences of the main elementary flows in RIs of Freshwater ecotoxicity

Elementary flow	1	2	3	4	5	6	7	total	% of total occurrence
copper, ion to water ground-, long-term	98	3546	2386	2194	2396	312	43	10975	29%
zinc, ion to water ground-, long-term	40	3530	2293	2166	2399	306	43	10777	58%
chromium vi to water ground-, long-term		26	591	1131	2211	265	39	4263	69%
vanadium, ion to water ground-, long-term	13	46	407	909	1825	211	38	3449	78%
nickel, ion to water ground-, long-term		11	496	696	1861	237	40	3341	87%
antimony to water ground-, long-term		12	374	119	260	52	2	819	89%
antimony to water surface water			83	56	219	38		396	90%
chromium vi to water surface water		12	44	62	103	113	2	336	91%

Table S 35. Occurrences of the main elementary flows in RIs of Land use

Elementary flow	1	2	3	4	5	6	7	8	9	10	total	% of total occurrence
transformation, to mineral extraction site to natural resource land	493	418	715	1449	1648	1623	1406	640	40	2	8434	16%
transformation, to annual crop, non-irrigated, intensive to natural resource land	1	404	706	849	1661	1784	1403	646	39	2	7495	31%
transformation, to industrial area to natural resource land	13	473	549	832	1333	1329	863	570	22	2	5986	42%
transformation, from annual crop to natural resource land		269	459	546	1274	1325	1296	624	38	2	5833	53%
transformation, from unspecified to natural resource land	62	295	432	669	1213	1180	770	493	14	2	5130	63%
transformation, from mineral extraction site to natural resource land	9	87	116	241	343	589	447	329	19	2	2182	68%
transformation, from annual crop, non-irrigated, intensive to natural resource land		193	212	168	53	315	485	373	20	2	1821	71%
transformation, to annual crop, non-irrigated, extensive to natural resource land		116		35	49	462	589	287	34	2	1574	74%

Table S 36. Occurrences of the main elementary flows in RIs of Water resource depletion

Elementary flow	1	2	3	total	% of total occurrence
water, river to natural resource in water	987	9458	688	11133	51%
water, well, in ground to natural resource in water	62	9443	688	10193	97%
water, lake to natural resource in water	9	19	688	716	100%

Table S 37. Occurrences of the main elementary flows in RIs of Mineral, fossil and renewable resource depletion

Elementary flow	1	2	3	4	5	6	7	8	total	% of total occurrence
indium, 0.005% in sulfide, in 0.003%, pb, zn, ag, cd, in ground to natural resource in ground		2596	5034	2149	558	289	27	3	10656	31%
nickel, 1.98% in silicates, 1.04% in crude ore, in ground to natural resource in ground	36	896	4508	1622	491	207	4		7764	53%
cadmium, 0.30% in sulfide, cd 0.18%, pb, zn, ag, in, in ground to natural resource in ground		1415	3869	1104	189	59	1		6637	72%
uranium, in ground to natural resource in ground	100	87	540	587	125	57	4		1500	76%
silver, ag 9.7e-4%, in mixed ore, in ground to natural resource in ground			18	600	430	213	6	3	1270	80%
copper, 0.99% in sulfide, cu 0.36% and mo 8.2e-3% in crude ore, in ground to natural resource in ground		21	39	314	456	210	2		1042	83%
tantalum, 81.9% in tantalite, 1.6e-4% in crude ore, in ground to natural resource in ground	12	71	241	317	16	123	1		781	85%
carbon, organic, in soil or biomass stock to natural resource in ground	41	98	154	273	13				579	87%

Annex C: Supplementary Information – Chapter 4

Annex C-1: Number of LCI per division

Table S 38. Number of LCI per division

Field of activity	Division	Name of division	Number of LCIs
Section A, Agriculture and forestry	1	Crop and animal production, hunting and related service activities	547
	2	Forestry and logging	85
Section B, Mining and quarrying	5	Mining of coal and lignite	26
	6	Extraction of crude petroleum and natural gas	42
	7	Mining of metal ores	114
	8	Other mining and quarrying	88
	9	Mining support service activities	10
Section C, Processed Biobased product	10	Manufacture of food products	128
	13	Manufacture of textiles	29
	16	Manufacture of wood and of products of wood and cork, except furniture; manufacture of articles of straw and plaiting materials	163
	17	Manufacture of paper and paper products	105
	18	Printing and reproduction of recorded media	5
	19.0	Biobased chemicals	52
Section C, Chemicals and Plastics	19.1	Manufacture of coke and refined petroleum products	98
	20	Manufacture of chemicals and chemical products	1345
	22	Manufacture of rubber and plastics products	51
Section C, Other non-metallic mineral products	23	Manufacture of other non-metallic mineral products	285
Section C, Metals and metal products	24	Manufacture of basic metals	234
	25	Manufacture of fabricated metal products, except machinery and equipment	330
Section C, Electronic and electronical equipment	26	Manufacture of computer, electronic and optical products	255
	27	Manufacture of electrical equipment	100

Section C, Machinery and transport equipment	28	Manufacture of machinery and equipment n.e.c.	276
	29	Manufacture of motor vehicles, trailers and semi-trailers	38
	30	Manufacture of other transport equipment	41
Section D, Electricity power generation	35.1	Electric power generation, transmission and distribution	2788
Section D, Manufacture of gas	35.2	Manufacture of gas; distribution of gaseous fuels through mains	90
Section D, Steam and air conditioning supply	35.3	Steam and air conditioning supply	407
Section E, Sewerage and Waste treatment	37	Sewerage	64
	38	Waste collection, treatment and disposal activities; materials recovery	1074
	39	Remediation activities and other waste management services	12
Section F, Construction	41	Construction of buildings	102
	42	Civil engineering	381
	43	Specialized construction activities	78
Section H, Transport land	49	Land transport and transport via pipelines Transport	179
total			9622

Annex C-2: Impact categories sorted by environmental issues

Table S 39. Identification key for impact categories classification

Environmental issue	Key	number of categories
Land occupation/transformation	1	21
Climate change	2	17
Resources and energy use	3	27
Eutrophication	4	20
Acidification	5	15
Ozone depletion	6	14
Photochemical oxidant formation	7	11
Particulate matter formation	8	12
Ecotoxicity	9	47
Human toxicity	10	28
Ionizing radiation	11	14
Water depletion	12	6
total		232

Table S 40. Classification of impact categories by environmental issues

Impact category	Environmental issue
Eco_Scarc_2013_V1.01_Land use	1
ILCD_Mid+_V1.05_Land use	1
Impact_2002+_V2.12_Land occupation	1
ReCiPe_End_E_V1.11_End_Agricultural land occupation	1
ReCiPe_End_E_V1.11_End_Natural land transformation	1
ReCiPe_End_E_V1.11_End_Urban land occupation	1
ReCiPe_End_H_V1.11_End_Agricultural land occupation	1
ReCiPe_End_H_V1.11_End_Natural land transformation	1
ReCiPe_End_H_V1.11_End_Urban land occupation	1
ReCiPe_End_I_V1.11_End_Agricultural land occupation	1
ReCiPe_End_I_V1.11_End_Natural land transformation	1
ReCiPe_End_I_V1.11_End_Urban land occupation	1
ReCiPe_Mid_E_V1.11_Agricultural land occupation	1
ReCiPe_Mid_E_V1.11_Natural land transformation	1
ReCiPe_Mid_E_V1.11_Urban land occupation	1
ReCiPe_Mid_H_V1.11_Agricultural land occupation	1
ReCiPe_Mid_H_V1.11_Natural land transformation	1
ReCiPe_Mid_H_V1.11_Urban land occupation	1
ReCiPe_Mid_I_V1.11_Agricultural land occupation	1
ReCiPe_Mid_I_V1.11_Natural land transformation	1
ReCiPe_Mid_I_V1.11_Urban land occupation	1
BEES_V4.05_Global warming	2
CML-IA_baseline_V3.02_Global warming (GWP100a)	2
Eco_Scarc_2013_V1.01_Global warming	2
EDIP_2003_V1.05_Global warming 100a	2
EPD_2013_V1.01_Global warming (GWP100a)	2
ILCD_Mid+_V1.05_Climate change	2
Impact_2002+_V2.12_Global warming	2
ReCiPe_End_E_V1.11_End_Climate change Ecosystems	2
ReCiPe_End_E_V1.11_End_Climate change Human Health	2
ReCiPe_End_H_V1.11_End_Climate change Ecosystems	2
ReCiPe_End_H_V1.11_End_Climate change Human Health	2
ReCiPe_End_I_V1.11_End_Climate change Ecosystems	2
ReCiPe_End_I_V1.11_End_Climate change Human Health	2
ReCiPe_Mid_E_V1.11_Climate change	2
ReCiPe_Mid_H_V1.11_Climate change	2
ReCiPe_Mid_I_V1.11_Climate change	2
TRACI_2.1_V1.02_Global warming	2
BEES_V4.05_Natural resource depletion	3
CML-IA_baseline_V3.02_Abiotic depletion	3

CML-IA_baseline_V3.02_Abiotic depletion (fossil fuels)	3
Eco_Scarc_2013_V1.01_Energy resources	3
Eco_Scarc_2013_V1.01_Heavy metals into soil	3
Eco_Scarc_2013_V1.01_Mineral resources	3
EDIP_2003_V1.05_Resources (all)	3
EPD_2013_V1.01_Abiotic depletion (optional)	3
EPS_2000_V2.08_Crop growth capacity	3
EPS_2000_V2.08_Depletion of reserves	3
EPS_2000_V2.08_Wood growth capacity	3
ILCD_Mid+_V1.05_Mineral, fossil & ren resource depletion	3
Impact_2002+_V2.12_Mineral extraction	3
Impact_2002+_V2.12_Non-renewable energy	3
ReCiPe_End_E_V1.11_End_Fossil depletion	3
ReCiPe_End_E_V1.11_End_Metal depletion	3
ReCiPe_End_H_V1.11_End_Fossil depletion	3
ReCiPe_End_H_V1.11_End_Metal depletion	3
ReCiPe_End_I_V1.11_End_Fossil depletion	3
ReCiPe_End_I_V1.11_End_Metal depletion	3
ReCiPe_Mid_E_V1.11_Fossil depletion	3
ReCiPe_Mid_E_V1.11_Metal depletion	3
ReCiPe_Mid_H_V1.11_Fossil depletion	3
ReCiPe_Mid_H_V1.11_Metal depletion	3
ReCiPe_Mid_I_V1.11_Fossil depletion	3
ReCiPe_Mid_I_V1.11_Metal depletion	3
TRACI_2.1_V1.02_Fossil fuel depletion	3
BEES_V4.05_Eutrophication	4
CML-IA_baseline_V3.02_Eutrophication	4
EDIP_2003_V1.05_Aquatic eutrophication EP(N)	4
EDIP_2003_V1.05_Aquatic eutrophication EP(P)	4
EDIP_2003_V1.05_Terrestrial eutrophication	4
EPD_2013_V1.01_Eutrophication	4
ILCD_Mid+_V1.05_Freshwater eutrophication	4
ILCD_Mid+_V1.05_Marine eutrophication	4
ILCD_Mid+_V1.05_Terrestrial eutrophication	4
Impact_2002+_V2.12_Aquatic eutrophication	4
ReCiPe_End_E_V1.11_End_Freshwater eutrophication	4
ReCiPe_End_H_V1.11_End_Freshwater eutrophication	4
ReCiPe_End_I_V1.11_End_Freshwater eutrophication	4
ReCiPe_Mid_E_V1.11_Freshwater eutrophication	4
ReCiPe_Mid_E_V1.11_Marine eutrophication	4
ReCiPe_Mid_H_V1.11_Freshwater eutrophication	4
ReCiPe_Mid_H_V1.11_Marine eutrophication	4
ReCiPe_Mid_I_V1.11_Freshwater eutrophication	4
ReCiPe_Mid_I_V1.11_Marine eutrophication	4
TRACI_2.1_V1.02_Eutrophication	4
BEES_V4.05_Acidification	5
CML-IA_baseline_V3.02_Acidification	5
EDIP_2003_V1.05_Acidification	5
EPD_2013_V1.01_Acidification (fate not incl.)	5
EPS_2000_V2.08_Soil acidification	5
ILCD_Mid+_V1.05_Acidification	5
Impact_2002+_V2.12_Aquatic acidification	5
Impact_2002+_V2.12_Terrestrial acid/nutri	5
ReCiPe_End_E_V1.11_End_Terrestrial acidification	5
ReCiPe_End_H_V1.11_End_Terrestrial acidification	5
ReCiPe_End_I_V1.11_End_Terrestrial acidification	5
ReCiPe_Mid_E_V1.11_Terrestrial acidification	5
ReCiPe_Mid_H_V1.11_Terrestrial acidification	5
ReCiPe_Mid_I_V1.11_Terrestrial acidification	5
TRACI_2.1_V1.02_Acidification	5
BEES_V4.05_Ozone depletion	6
CML-IA_baseline_V3.02_Ozone layer depletion (ODP)	6
Eco_Scarc_2013_V1.01_Ozone layer depletion	6
EDIP_2003_V1.05_Ozone depletion	6
EPD_2013_V1.01_Ozone layer depletion (ODP) (optional)	6
ILCD_Mid+_V1.05_Ozone depletion	6

Impact_2002+_V2.12_Ozone layer depletion	6
ReCiPe_End_E_V1.11_End_Ozone depletion	6
ReCiPe_End_H_V1.11_End_Ozone depletion	6
ReCiPe_End_I_V1.11_End_Ozone depletion	6
ReCiPe_Mid_E_V1.11_Ozone depletion	6
ReCiPe_Mid_H_V1.11_Ozone depletion	6
ReCiPe_Mid_I_V1.11_Ozone depletion	6
TRACI_2.1_V1.02_Ozone depletion	6
CML-IA_baseline_V3.02_Photochemical oxidation	7
EDIP_2003_V1.05_Ozone formation (Human)	7
EDIP_2003_V1.05_Ozone formation (Vegetation)	7
EPD_2013_V1.01_Photochemical oxidation	7
ILCD_Mid+_V1.05_Photochemical ozone formation	7
ReCiPe_End_E_V1.11_End_Photochemical oxidant formation	7
ReCiPe_End_H_V1.11_End_Photochemical oxidant formation	7
ReCiPe_End_I_V1.11_End_Photochemical oxidant formation	7
ReCiPe_Mid_E_V1.11_Photochemical oxidant formation	7
ReCiPe_Mid_H_V1.11_Photochemical oxidant formation	7
ReCiPe_Mid_I_V1.11_Photochemical oxidant formation	7
BEES_V4.05_Smog	8
Eco_Scarc_2013_V1.01_Main air pollutants and PM	8
ILCD_Mid+_V1.05_Particulate matter	8
Impact_2002+_V2.12_Respiratory inorganics	8
ReCiPe_End_E_V1.11_End_Particulate matter formation	8
ReCiPe_End_H_V1.11_End_Particulate matter formation	8
ReCiPe_End_I_V1.11_End_Particulate matter formation	8
ReCiPe_Mid_E_V1.11_Particulate matter formation	8
ReCiPe_Mid_H_V1.11_Particulate matter formation	8
ReCiPe_Mid_I_V1.11_Particulate matter formation	8
TRACI_2.1_V1.02_Respiratory effects	8
TRACI_2.1_V1.02_Smog	8
BEES_V4.05_Ecotoxicity	9
BEES_V4.05_Habitat alteration	9
CML-IA_baseline_V3.02_Fresh water aquatic ecotox.	9
CML-IA_baseline_V3.02_Marine aquatic ecotoxicity	9
CML-IA_baseline_V3.02_Terrestrial ecotoxicity	9
Eco_Scarc_2013_V1.01_Heavy metals into water	9
Eco_Scarc_2013_V1.01_Pesticides into soil	9
Eco_Scarc_2013_V1.01_POP into water	9
Eco_Scarc_2013_V1.01_Water pollutants	9
EDIP_2003_V1.05_Bulk waste	9
EDIP_2003_V1.05_Ecotoxicity soil chronic	9
EDIP_2003_V1.05_Ecotoxicity water acute	9
EDIP_2003_V1.05_Ecotoxicity water chronic	9
EDIP_2003_V1.05_Hazardous waste	9
EDIP_2003_V1.05_Slags/ashes	9
EPS_2000_V2.08_Fish and meat production	9
EPS_2000_V2.08_Nuisance	9
EPS_2000_V2.08_Severe nuisance	9
EPS_2000_V2.08_Species extinction	9
ILCD_Mid+_V1.05_Freshwater ecotoxicity	9
Impact_2002+_V2.12_Aquatic ecotoxicity	9
Impact_2002+_V2.12_Terrestrial ecotoxicity	9
ReCiPe_End_E_V1.11_Damage_Ecosystems	9
ReCiPe_End_E_V1.11_Damage_Ressources	9
ReCiPe_End_E_V1.11_End_Freshwater ecotoxicity	9
ReCiPe_End_E_V1.11_End_Marine ecotoxicity	9
ReCiPe_End_E_V1.11_End_Terrestrial ecotoxicity	9
ReCiPe_End_H_V1.11_Damage_Ecosystems	9
ReCiPe_End_H_V1.11_Damage_Ressources	9
ReCiPe_End_H_V1.11_End_Freshwater ecotoxicity	9
ReCiPe_End_H_V1.11_End_Marine ecotoxicity	9
ReCiPe_End_H_V1.11_End_Terrestrial ecotoxicity	9
ReCiPe_End_I_V1.11_Damage_Ecosystems	9
ReCiPe_End_I_V1.11_Damage_Ressources	9
ReCiPe_End_I_V1.11_End_Freshwater ecotoxicity	9

ReCiPe_End_I_V1.11_End_Marine ecotoxicity	9
ReCiPe_End_I_V1.11_End_Terrestrial ecotoxicity	9
ReCiPe_Mid_E_V1.11_Freshwater ecotoxicity	9
ReCiPe_Mid_E_V1.11_Marine ecotoxicity	9
ReCiPe_Mid_E_V1.11_Terrestrial ecotoxicity	9
ReCiPe_Mid_H_V1.11_Freshwater ecotoxicity	9
ReCiPe_Mid_H_V1.11_Marine ecotoxicity	9
ReCiPe_Mid_H_V1.11_Terrestrial ecotoxicity	9
ReCiPe_Mid_I_V1.11_Freshwater ecotoxicity	9
ReCiPe_Mid_I_V1.11_Marine ecotoxicity	9
ReCiPe_Mid_I_V1.11_Terrestrial ecotoxicity	9
TRACI_2.1_V1.02_Ecotoxicity	9
BEES_V4.05_HH cancer	10
BEES_V4.05_HH criteria air pollutants	10
BEES_V4.05_HH noncancer	10
CML-IA_baseline_V3.02_Human toxicity	10
Eco_Scarc_2013_V1.01_Carcinogenic substances into air	10
Eco_Scarc_2013_V1.01_Heavy metals into air	10
EDIP_2003_V1.05_Human toxicity air	10
EDIP_2003_V1.05_Human toxicity soil	10
EDIP_2003_V1.05_Human toxicity water	10
EPS_2000_V2.08_Life expectancy	10
EPS_2000_V2.08_Morbidity	10
EPS_2000_V2.08_Severe morbidity	10
ILCD_Mid+_V1.05_Human toxicity, cancer effects	10
ILCD_Mid+_V1.05_Human toxicity, non-cancer effects	10
Impact_2002+_V2.12_Carcinogens	10
Impact_2002+_V2.12_Non-carcinogens	10
Impact_2002+_V2.12_Respiratory organics	10
ReCiPe_End_E_V1.11_Damage_Human Health	10
ReCiPe_End_E_V1.11_End_Human toxicity	10
ReCiPe_End_H_V1.11_Damage_Human Health	10
ReCiPe_End_H_V1.11_End_Human toxicity	10
ReCiPe_End_I_V1.11_Damage_Human Health	10
ReCiPe_End_I_V1.11_End_Human toxicity	10
ReCiPe_Mid_E_V1.11_Human toxicity	10
ReCiPe_Mid_H_V1.11_Human toxicity	10
ReCiPe_Mid_I_V1.11_Human toxicity	10
TRACI_2.1_V1.02_Carcinogenics	10
TRACI_2.1_V1.02_Non carcinogenics	10
Eco_Scarc_2013_V1.01_Non radioactive waste to deposit	11
Eco_Scarc_2013_V1.01_Radioactive substances into air	11
Eco_Scarc_2013_V1.01_Radioactive substances into water	11
Eco_Scarc_2013_V1.01_Radioactive waste to deposit	11
EDIP_2003_V1.05_Radioactive waste	11
ILCD_Mid+_V1.05_Ionizing radiation E (interim)	11
ILCD_Mid+_V1.05_Ionizing radiation HH	11
Impact_2002+_V2.12_Ionizing radiation	11
ReCiPe_End_E_V1.11_End_Ionising radiation	11
ReCiPe_End_H_V1.11_End_Ionising radiation	11
ReCiPe_End_I_V1.11_End_Ionising radiation	11
ReCiPe_Mid_E_V1.11_Ionising radiation	11
ReCiPe_Mid_H_V1.11_Ionising radiation	11
ReCiPe_Mid_I_V1.11_Ionising radiation	11
BEES_V4.05_Water intake	12
Eco_Scarc_2013_V1.01_Water resources	12
ILCD_Mid+_V1.05_Water resource depletion	12
ReCiPe_Mid_E_V1.11_Water depletion	12
ReCiPe_Mid_H_V1.11_Water depletion	12
ReCiPe_Mid_I_V1.11_Water depletion	12

Annex C-3: RIs medians and inter-quartiles of LCIA methods per field of activity

Table S 41. RIs medians of LCIA methods per fields of activity (1)

LCIA method	Section A_Agriculture and forestery	Section B_Mining and quarrying	Section C_Processed Biobased product	Section C_Chemicals and Plastics	Section C_Other non-metallic mineral products	Section C_Metals and metal products	Section C_Electronic and electronical equipment
BEES	1.67E-04	6.52E-03	3.45E-04	9.73E-04	1.42E-02	9.05E-03	1.29E-03
CML-IA	2.90E-04	1.07E-02	8.43E-04	1.93E-03	1.69E-02	1.65E-02	5.74E-03
ECO_Scarcity	4.93E-03	1.38E-02	1.88E-02	2.63E-03	2.14E-02	2.06E-02	4.25E-03
EDIP	1.36E-03	8.37E-03	1.59E-03	1.89E-03	1.61E-02	1.10E-02	2.72E-03
EPD	2.03E-04	3.77E-03	3.85E-04	8.56E-04	1.31E-02	8.20E-03	5.38E-03
EPS	1.29E-03	1.13E-02	1.07E-03	1.51E-03	1.46E-02	1.24E-02	4.67E-03
ILCD	1.11E-03	4.45E-03	1.17E-03	1.13E-03	1.50E-02	9.12E-03	2.12E-03
Impact_2002+	3.66E-03	1.14E-02	3.41E-03	1.53E-03	1.65E-02	9.76E-03	2.67E-03
ReCiPe_end_dam_E	9.03E-05	2.68E-03	1.59E-04	3.54E-04	8.33E-03	3.46E-03	7.30E-04
ReCiPe_end_dam_H	3.04E-04	2.36E-03	3.51E-04	4.05E-04	9.60E-03	2.95E-03	6.30E-04
ReCiPe_end_dam_I	2.92E-04	2.73E-03	3.66E-04	4.32E-04	1.00E-02	3.29E-03	8.97E-04
ReCiPe_end_imp_E	1.34E-03	1.20E-02	2.65E-03	1.36E-03	1.67E-02	1.12E-02	4.20E-03
ReCiPe_end_imp_H	1.51E-03	1.30E-02	4.56E-03	1.88E-03	1.68E-02	1.06E-02	3.78E-03
ReCiPe_end_imp_I	1.81E-03	1.18E-02	4.46E-03	1.91E-03	2.04E-02	1.45E-02	3.75E-03
ReCiPe_mid_E	1.10E-03	1.12E-02	2.65E-03	1.39E-03	1.69E-02	1.06E-02	4.20E-03
ReCiPe_mid_H	1.42E-03	1.31E-02	5.06E-03	1.80E-03	1.72E-02	1.06E-02	3.80E-03
ReCiPe_mid_I	1.42E-03	1.18E-02	4.58E-03	1.80E-03	2.07E-02	1.52E-02	3.96E-03
TRACI	1.57E-04	3.34E-03	2.57E-04	7.53E-04	1.18E-02	7.47E-03	9.50E-04

Table S 42. RIs medians of LCIA methods per fields of activity (2)

LCIA method	**Section C_Machinery and transport equipment**	**Section D_Electricity power generation**	**Section D_Manufacture of gas**	**Section D_Steam and air conditioning supply**	**Section E_Sewerage and Waste treatment**	**Section F_Construction**	**Section H_Transport land**
BEES	2.38E-02	5.12E-02	3.39E-02	6.15E-03	8.80E-03	1.58E-02	1.61E-02
CML-IA	7.98E-02	4.52E-02	3.19E-02	1.14E-02	9.79E-03	5.79E-02	1.67E-02
ECO_Scarcity	8.23E-02	7.83E-02	4.60E-02	8.03E-02	2.53E-02	6.81E-02	5.80E-02
EDIP	6.33E-02	4.11E-02	3.07E-02	3.12E-02	1.26E-02	4.51E-02	2.86E-02
EPD	4.42E-02	3.10E-02	1.93E-02	9.20E-03	7.39E-03	4.05E-02	1.37E-02
EPS	6.28E-02	2.91E-02	2.49E-02	2.64E-02	2.91E-03	5.21E-02	2.53E-02
ILCD	5.22E-02	5.07E-02	2.45E-02	1.98E-02	8.20E-03	4.01E-02	1.73E-02
Impact_2002+	3.29E-02	5.73E-02	5.91E-02	9.02E-02	1.02E-02	3.36E-02	3.67E-02
ReCiPe_end_dam_E	1.26E-02	1.85E-02	2.60E-02	5.17E-03	1.79E-03	1.18E-02	7.49E-03
ReCiPe_end_dam_H	9.82E-03	1.97E-02	2.60E-02	2.90E-02	8.09E-04	7.28E-03	7.36E-03
ReCiPe_end_dam_I	1.34E-02	2.19E-02	2.56E-02	1.54E-02	7.38E-04	8.48E-03	9.22E-03
ReCiPe_end_imp_E	4.02E-02	4.53E-02	4.55E-02	1.04E-01	7.67E-03	4.45E-02	4.18E-02
ReCiPe_end_imp_H	3.99E-02	5.57E-02	5.75E-02	1.04E-01	1.75E-02	4.34E-02	4.48E-02
ReCiPe_end_imp_I	4.81E-02	5.42E-02	5.32E-02	1.03E-01	1.76E-02	4.43E-02	4.54E-02
ReCiPe_mid_E	4.03E-02	7.26E-02	4.32E-02	1.05E-01	1.23E-02	4.36E-02	5.29E-02
ReCiPe_mid_H	3.99E-02	7.55E-02	5.48E-02	1.05E-01	1.77E-02	4.34E-02	5.29E-02
ReCiPe_mid_I	4.81E-02	7.52E-02	5.28E-02	1.05E-01	1.77E-02	4.43E-02	5.16E-02
TRACI	1.72E-02	3.03E-02	3.42E-02	8.69E-03	6.33E-03	1.20E-02	1.32E-02

Table S 43. RIs inter-quartiles of LCIA methods per fields of activity (1)

LCIA method	Section A_Agriculture and forestery	Section B_Mining and quarrying	Section C_Processed Biobased product	Section C_Chemicals and Plastics	Section C_Other non-metallic mineral products	Section C_Metals and metal products	Section C_Electronic and electronical equipment
BEES	2.62E+02	1.33E+02	7.74E+01	2.21E+02	1.58E+01	1.86E+01	5.50E+01
CML-IA	2.86E+02	1.76E+02	5.88E+01	1.71E+02	1.86E+01	2.64E+01	1.74E+02
ECO_Scarcity	2.62E+01	1.82E+02	2.75E+01	3.49E+02	1.03E+01	2.17E+01	4.67E+01
EDIP	7.00E+01	1.31E+02	2.38E+01	2.47E+02	1.44E+01	2.34E+01	7.52E+01
EPD	4.35E+02	1.89E+02	5.78E+01	1.48E+02	1.48E+01	2.68E+01	1.66E+02
EPS	1.47E+02	7.91E+01	4.89E+01	1.12E+02	1.21E+01	1.61E+01	6.89E+01
ILCD	6.29E+01	1.27E+02	5.19E+01	2.91E+02	1.71E+01	1.84E+01	7.79E+01
Impact_2002+	5.26E+01	2.02E+02	3.01E+01	3.49E+02	1.63E+01	2.28E+01	5.71E+01
ReCiPe_end_dam_E	3.86E+02	2.05E+02	1.14E+02	2.68E+02	2.88E+01	2.19E+01	1.10E+02
ReCiPe_end_dam_H	1.54E+02	1.48E+02	1.07E+02	2.10E+02	3.08E+01	2.95E+01	6.37E+01
ReCiPe_end_dam_I	1.82E+02	9.12E+01	7.79E+01	1.99E+02	2.84E+01	3.48E+01	5.49E+01
ReCiPe_end_imp_E	1.17E+02	1.00E+02	8.90E+01	3.86E+02	1.31E+01	3.43E+01	3.35E+01
ReCiPe_end_imp_H	3.74E+01	1.10E+02	8.87E+01	3.30E+02	1.30E+01	3.32E+01	1.62E+01
ReCiPe_end_imp_I	2.54E+01	1.10E+02	6.92E+01	3.21E+02	1.50E+01	3.45E+01	1.60E+01
ReCiPe_mid_E	1.26E+02	1.10E+02	1.02E+02	3.89E+02	1.34E+01	2.69E+01	3.35E+01
ReCiPe_mid_H	4.30E+01	1.11E+02	9.87E+01	3.25E+02	1.34E+01	2.72E+01	1.65E+01
ReCiPe_mid_I	4.46E+01	1.10E+02	1.02E+02	3.49E+02	1.51E+01	2.57E+01	1.64E+01
TRACI	2.04E+02	1.53E+02	5.57E+01	2.82E+02	2.23E+01	1.65E+01	8.11E+01

Table S 44. RIs inter-quartiles of LCIA methods per fields of activity (2)

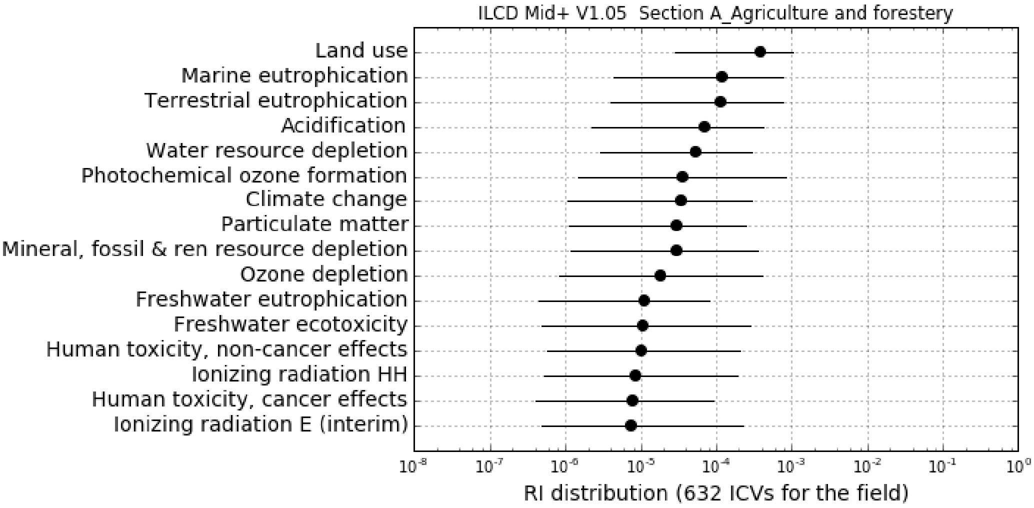
LCIA method	Section C_Machinery and transport equipment	Section D_Electricity power generation	Section D_Manufacture of gas	Section D_Steam and air conditioning supply	Section E_Sewerage and Waste treatment	Section F_Construction	Section H_Transport land
BEES	7.21E+00	6.81E+00	5.57E+00	1.80E+00	1.06E+01	9.36E+00	9.43E+01
CML-IA	1.20E+01	1.32E+01	6.81E+00	1.65E+00	1.84E+01	1.42E+01	1.78E+02
ECO_Scarcity	1.03E+01	1.06E+01	4.20E+00	1.77E+00	3.36E+01	8.39E+00	6.03E+02
EDIP	1.13E+01	9.83E+00	6.92E+00	2.83E+00	1.89E+01	1.19E+01	6.89E+01
EPD	1.02E+01	1.31E+01	1.08E+01	1.55E+00	2.04E+01	1.52E+01	1.72E+02
EPS	8.46E+00	1.84E+01	5.57E+00	2.52E+00	2.71E+00	8.80E+00	2.37E+02
ILCD	1.23E+01	1.15E+01	7.19E+00	1.60E+00	1.20E+01	8.33E+00	3.35E+02
Impact_2002+	9.15E+00	1.80E+01	5.78E+00	2.27E+00	3.51E+00	7.68E+00	5.19E+02
ReCiPe_end_dam_E	1.34E+01	2.68E+01	6.41E+00	2.32E+00	9.71E+00	1.12E+01	3.50E+02
ReCiPe_end_dam_H	6.37E+00	3.72E+01	4.48E+00	2.63E+00	3.93E+00	9.43E+00	3.64E+02
ReCiPe_end_dam_I	8.59E+00	2.67E+01	6.12E+00	2.77E+00	6.52E+00	1.08E+01	3.75E+02
ReCiPe_end_imp_E	1.46E+01	6.93E+00	4.68E+00	2.68E+00	3.03E+00	9.36E+00	7.09E+02
ReCiPe_end_imp_H	1.32E+01	8.43E+00	4.22E+00	2.59E+00	5.64E+00	8.86E+00	6.46E+02
ReCiPe_end_imp_I	1.35E+01	1.06E+01	5.02E+00	2.62E+00	5.81E+00	8.65E+00	6.53E+02
ReCiPe_mid_E	1.41E+01	4.51E+00	4.50E+00	2.65E+00	2.38E+01	9.18E+00	7.09E+02
ReCiPe_mid_H	1.27E+01	4.59E+00	4.96E+00	2.57E+00	7.98E+00	8.77E+00	6.48E+02
ReCiPe_mid_I	1.31E+01	4.47E+00	4.85E+00	2.64E+00	7.63E+00	8.60E+00	6.54E+02
TRACI	7.92E+00	1.30E+01	6.82E+00	1.59E+00	1.06E+01	8.79E+00	4.22E+02

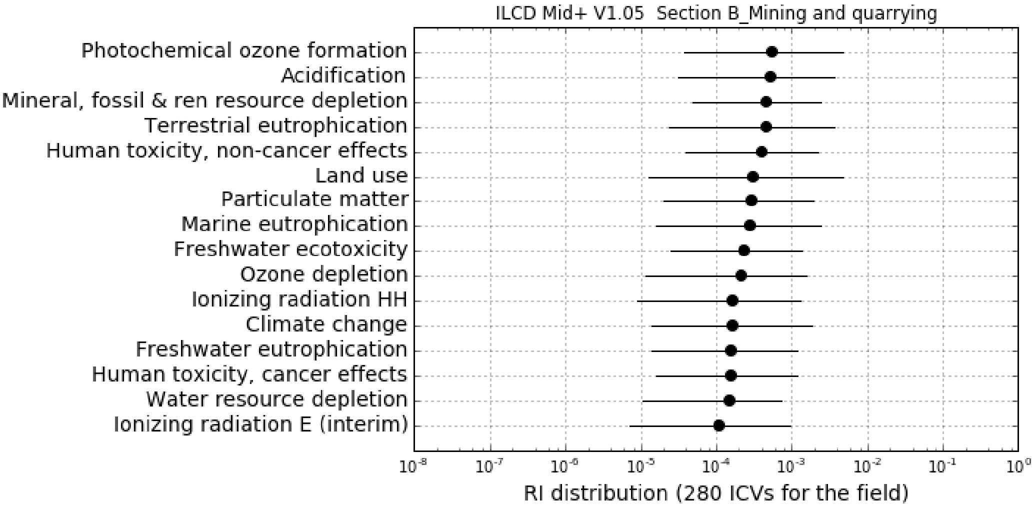
Annex C-4: RIs distributions per field of activity for the ILCD method

The Table S 45 presents descriptive statistics of RI distributions of the ILCD impact categories per field of activity. The respective RI distributions are plotted on the following figures.

Table S 45. Descriptive statistics of RI distributions of the ILCD impact categories per field of activity

Field of activity	median geometric mean	Ratio median max and median min	median max	median min	Quartile 1 min	Qaurtile 3 max
Database	5.80E-04	3.70E+00	1.02E-03	2.76E-04	1.85E-05	7.17E-03
Section A, Agriculture and forestry	2.90E-05	4.87E+01	3.60E-04	7.39E-06	4.14E-07	1.00E-03
Section B, Mining and quarrying	2.84E-04	5.22E+00	5.78E-04	1.11E-04	8.55E-06	5.76E-03
Section C, Processed Biobased product	7.57E-05	9.86E+00	2.86E-04	2.90E-05	2.07E-06	2.09E-03
Section C, Chemicals and Plastics	8.44E-05	4.47E+00	1.75E-04	3.91E-05	1.88E-06	2.24E-03
Section C, Other non-metallic mineral products	1.97E-03	1.10E+01	6.21E-03	5.65E-04	6.55E-05	1.20E-02
Section C, Metals and metal products	1.13E-03	5.65E+00	2.61E-03	4.62E-04	6.16E-05	6.61E-03
Section C, Electronic and electronical equipment	1.86E-04	1.00E+01	7.38E-04	7.37E-05	6.28E-06	6.73E-03
Section C, Machinery and transport equipment	3.62E-03	8.34E+00	1.10E-02	1.33E-03	3.11E-04	3.80E-02
Section D, Electricity power generation	2.73E-03	1.22E+01	9.26E-03	7.58E-04	1.11E-04	2.19E-02
Section D, Manufacture of gas	2.20E-03	3.29E+01	1.47E-02	4.46E-04	7.39E-05	5.29E-02
Section D, Steam and air conditioning supply	9.64E-04	8.84E+01	8.17E-03	9.24E-05	5.08E-05	1.25E-02
Section E, Sewerage and Waste treatment	2.64E-04	1.18E+01	9.21E-04	7.83E-05	1.02E-05	4.15E-03
Section F, Construction	2.40E-03	1.28E+01	8.51E-03	6.64E-04	1.66E-04	3.40E-02
Section H, Transport land	2.29E-03	1.59E+01	7.50E-03	4.71E-04	4.07E-06	1.46E-02





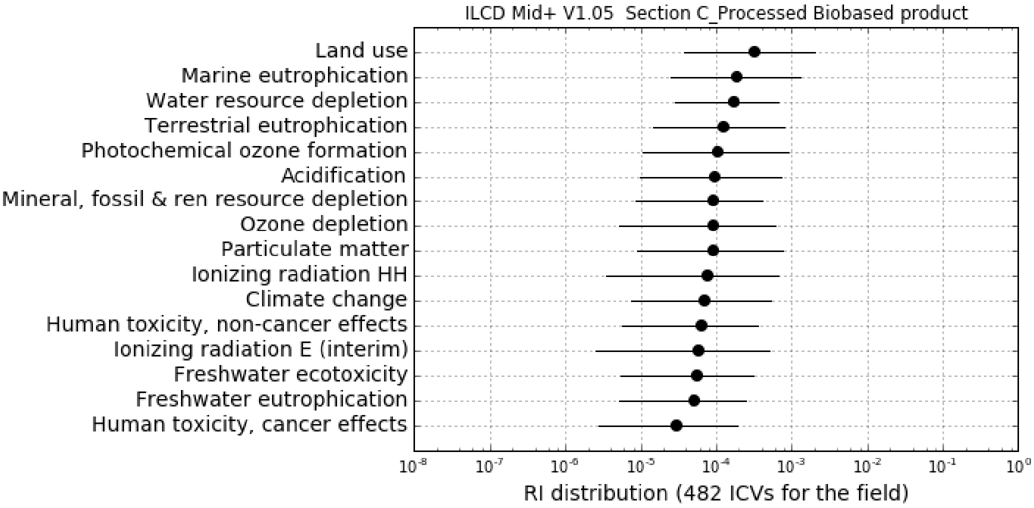
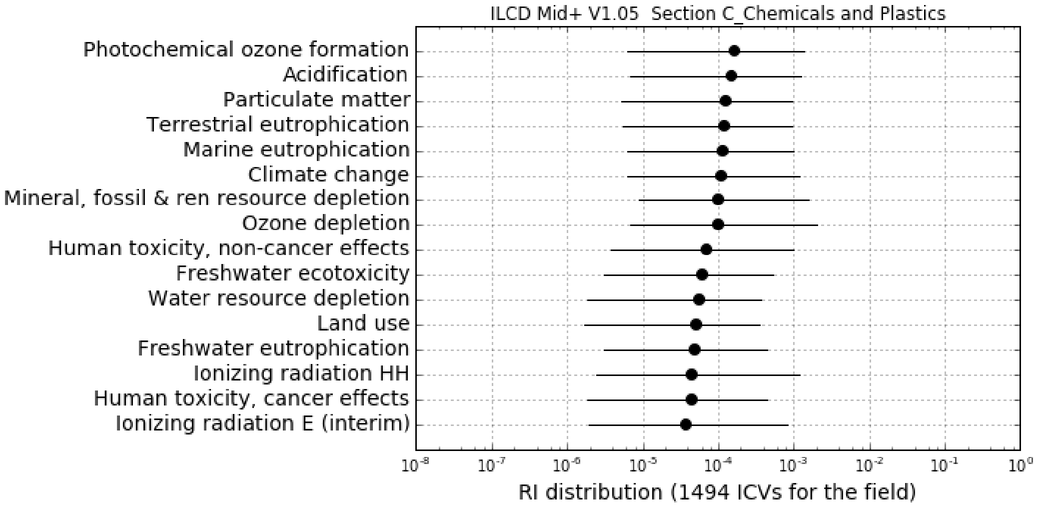
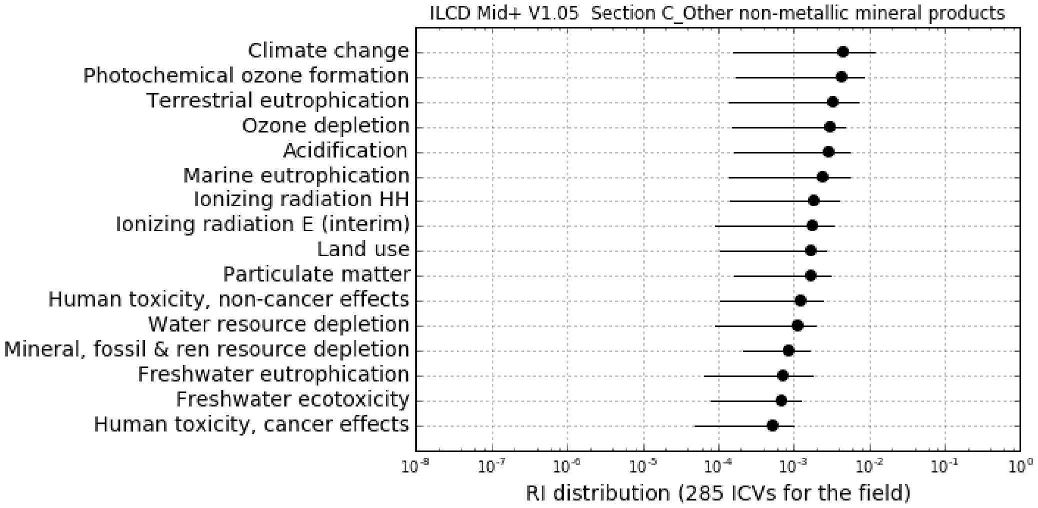


Figure S 15. Distributions of impact category RIs for Sections A, B and C (Section C: Processed Biobased products)





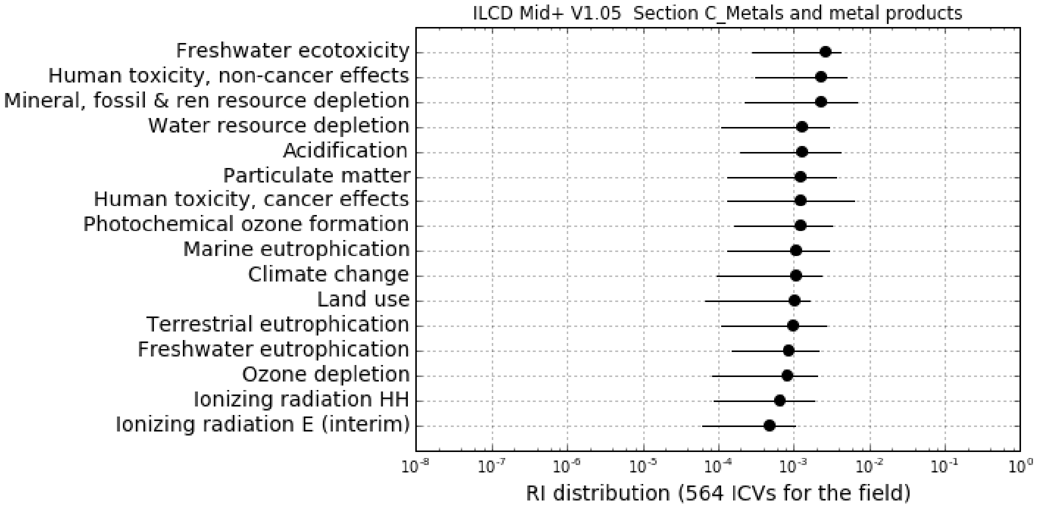
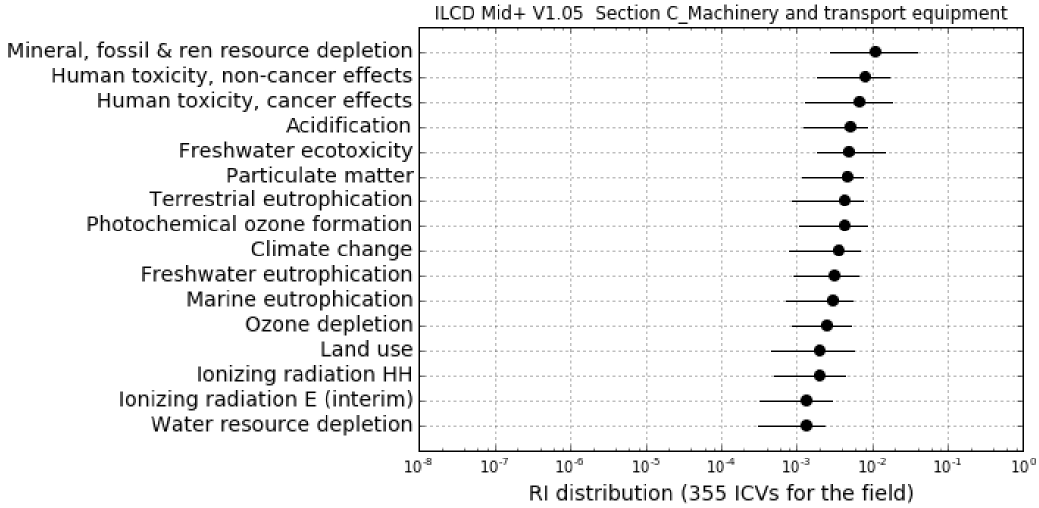
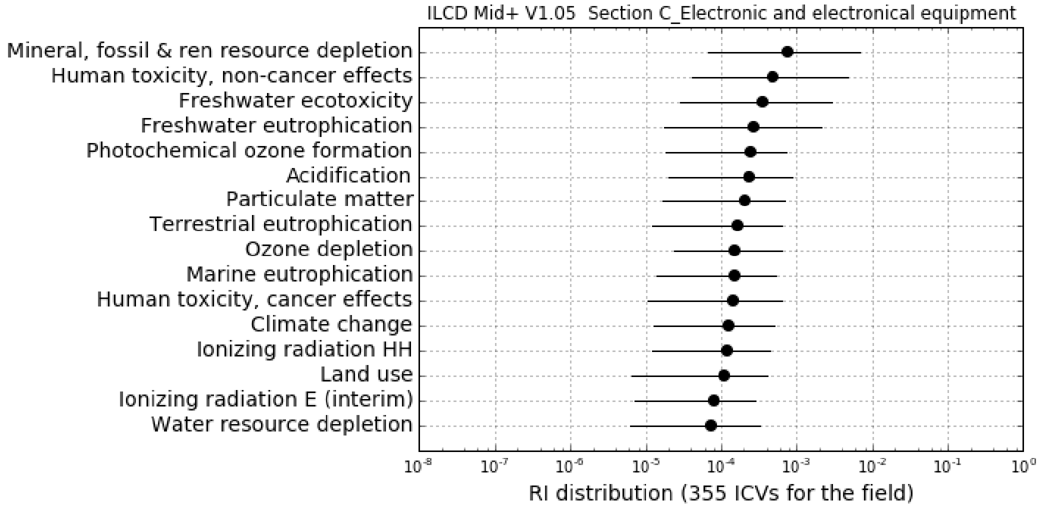


Figure S 16. Distributions of impact category RIs for Sections C (Chemicals and Plastics, Other non-metallic mineral products, Metals and metal products)





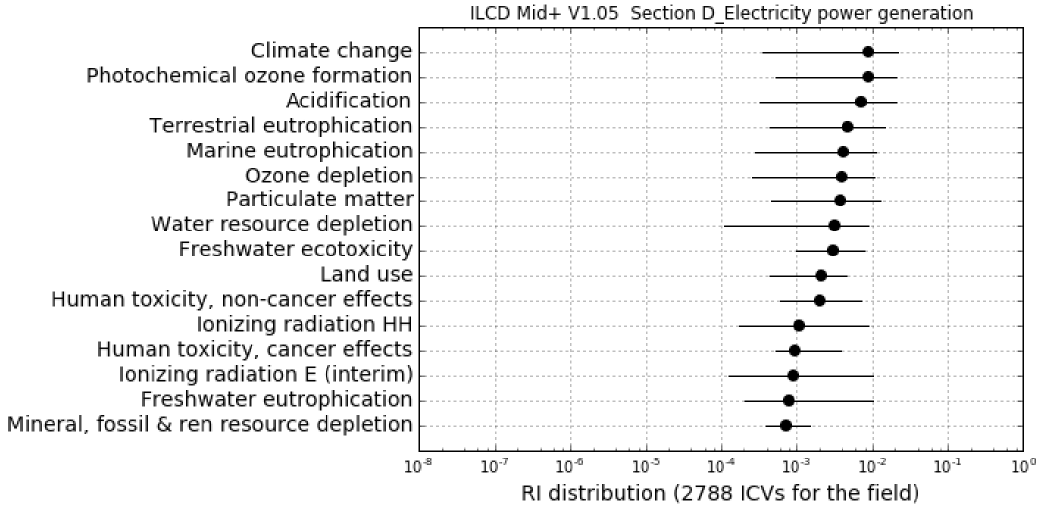
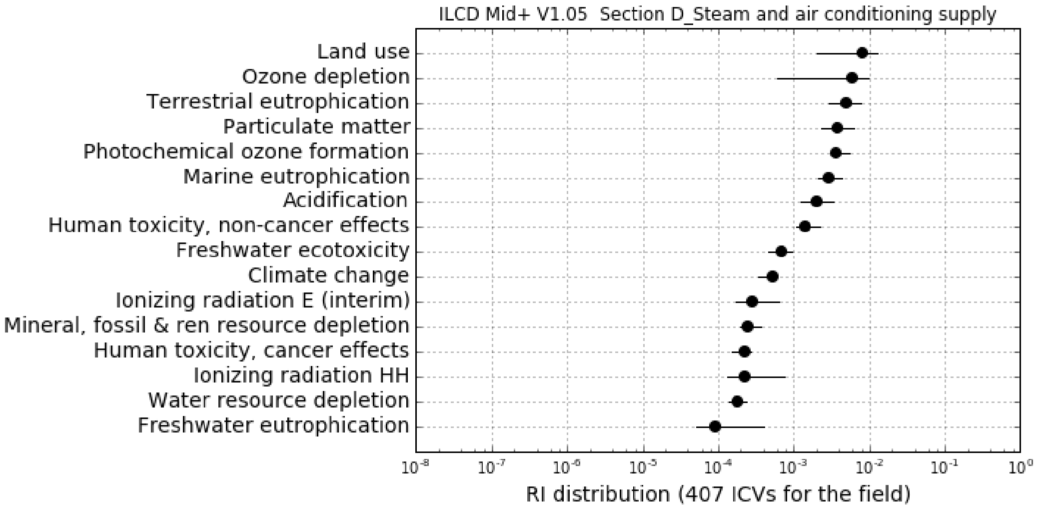
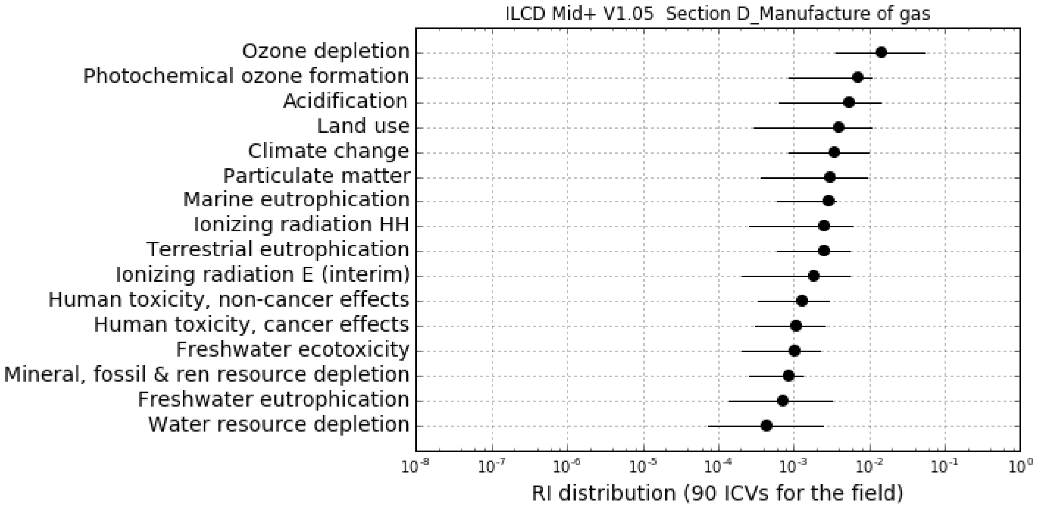


Figure S 17. Distributions of impact category RIs for Sections C (Machinery and transport equipment, Electronic and electronical equipment) and Section D (Electricity power generation)





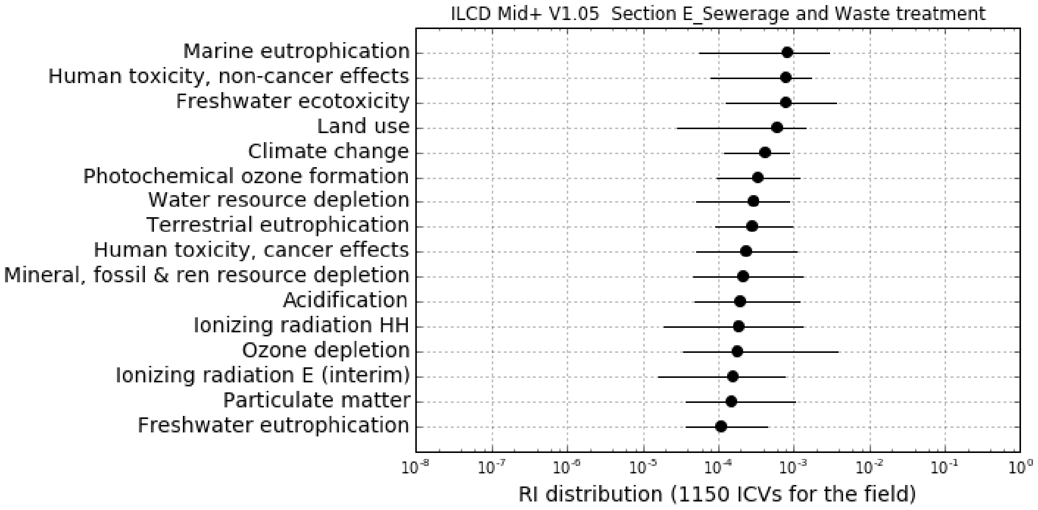


Figure S 18. Distributions of impact category RIs for Sections D (Steam and air conditioning supply, Manufacture of gas) and Section E

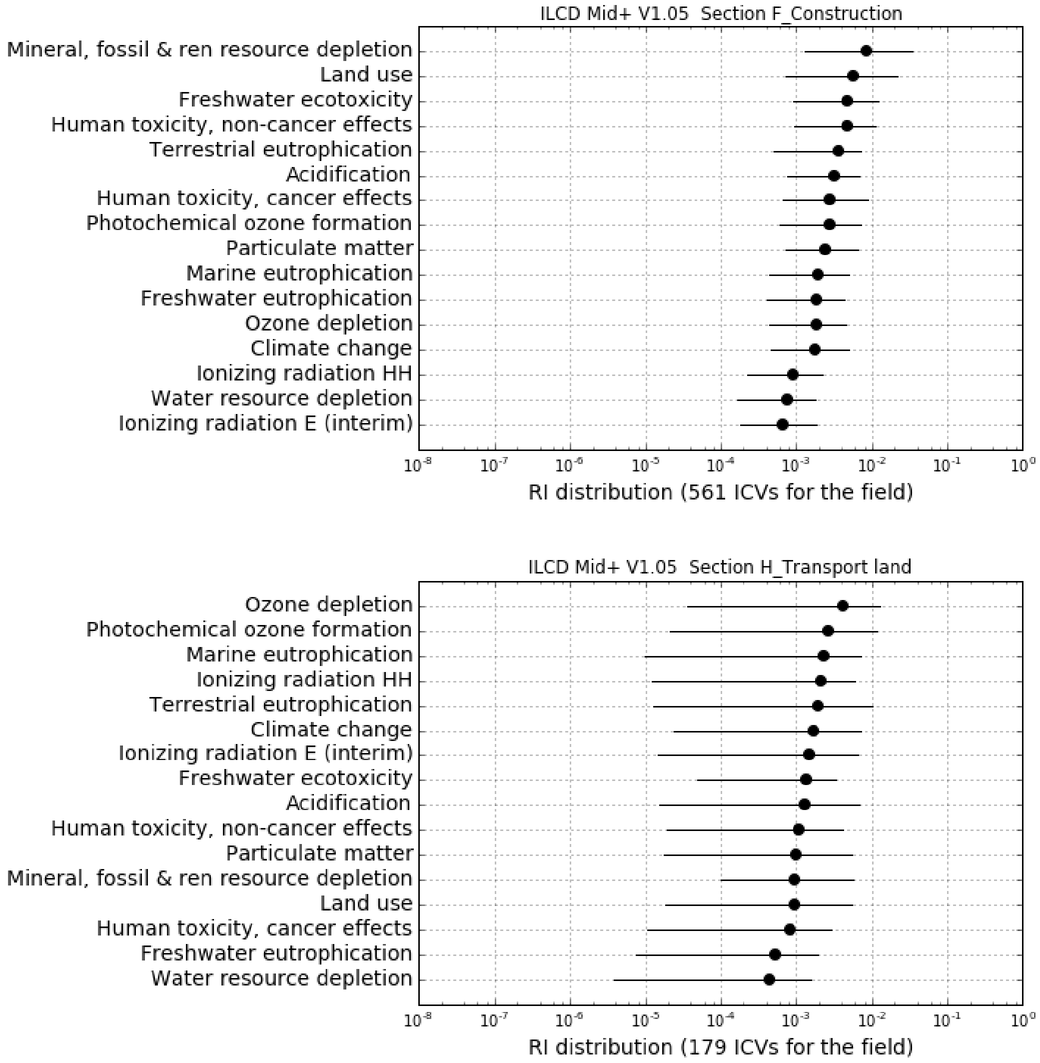


Figure S 19. Distributions of impact category RIs for Sections F and H

Annex D: Supplementary Information – Chapter 5

Annex D-1: Contribution analysis

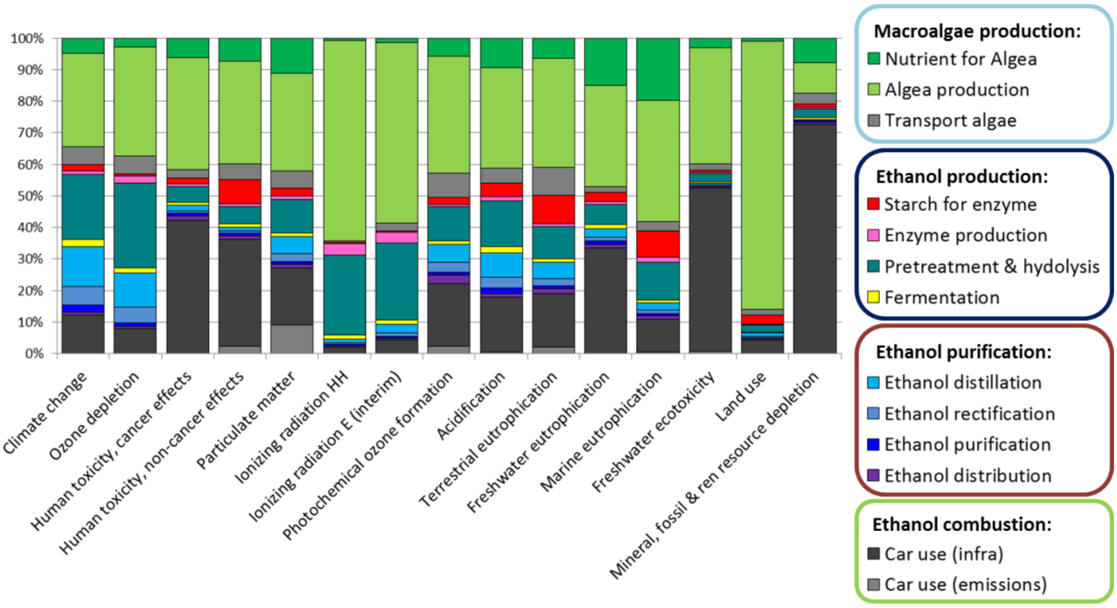


Figure S 20. Contribution analysis regarding LCI steps

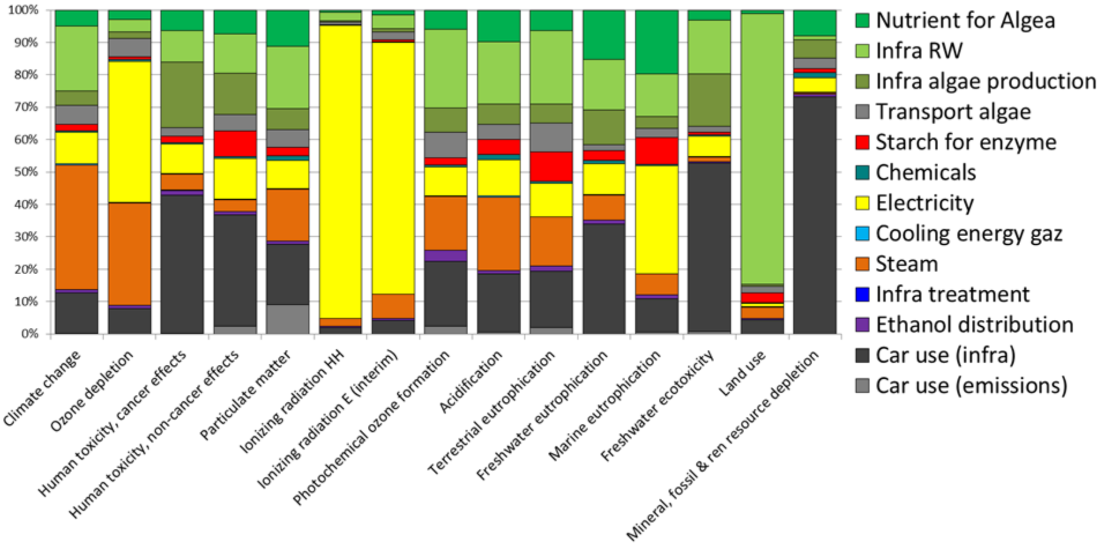


Figure S 21. Contribution analysis regarding infrastructure, energy and main inputs

Annex D-2: Impact category RI screening

The following figures present the screening of the RIs of the impact categories from classic LCIA methods. The Figure S 22 corresponds to the screenings of the global LCI. Then, RIs of the four sub-systems are presented. Only the first thirty impact categories with the highest RIs are plotted.

Regarding subsystems of the LCI, the macro-algae production step results (Figure S 23) are quite similar to the entire LCI. Urban land occupations are ranked first but ionizing radiations are ranked before toxicities. The impact category “Pesticide into soil” from Ecological scarcity is the main relevant impact category for ethanol production (Figure S 24). Elementary flows that are linked to conventional maize production, used for the enzyme production step, are the one that support this RI. Other ecotoxicity impact categories are following. Ionizing radiation and ozone depletion impact categories are the other main environmental issues that are put forward by our methodology.

With ecotoxicities and ozone depletion categories, resource depletions are considered valuable to study for the ethanol purification (Figure S 25). The use of natural gas for steam production leads the LCI on dimensions considered as critical for those impact categories. Finally, screening of impact categories for the combustion of ethanol (Figure S 26) shows toxicities and metal depletion as the main relevant impact categories.

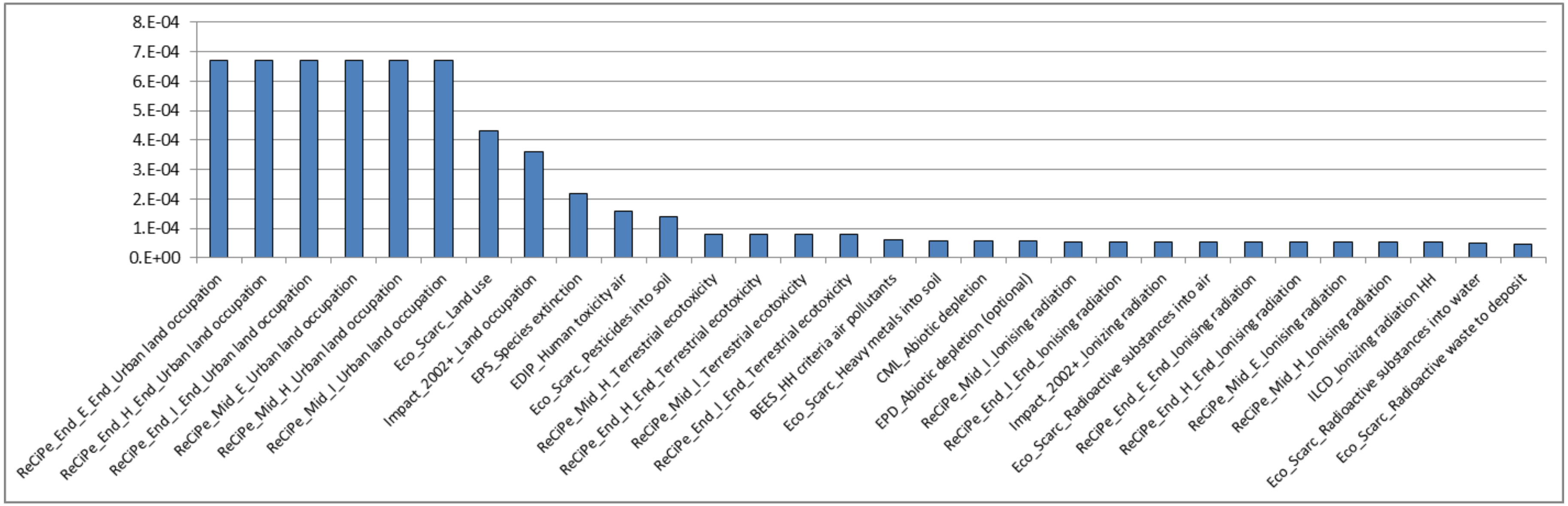


Figure S 22. Impact category RI screening for the global LCI

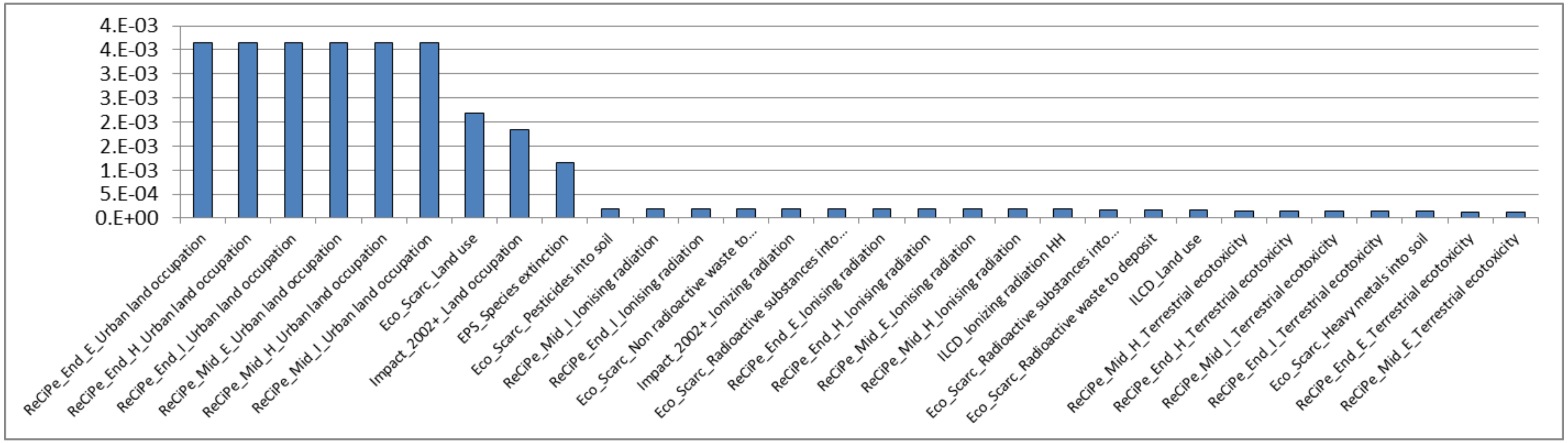


Figure S 23. Impact category RI screening for the macro-algae production step

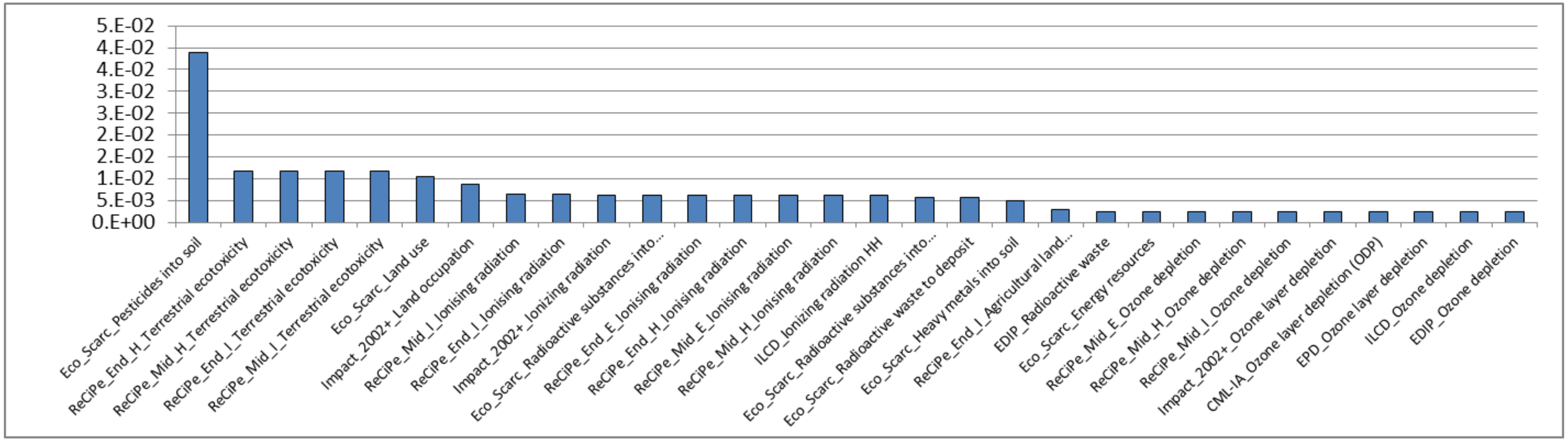


Figure S 24. Impact category RI screening for the ethanol production step

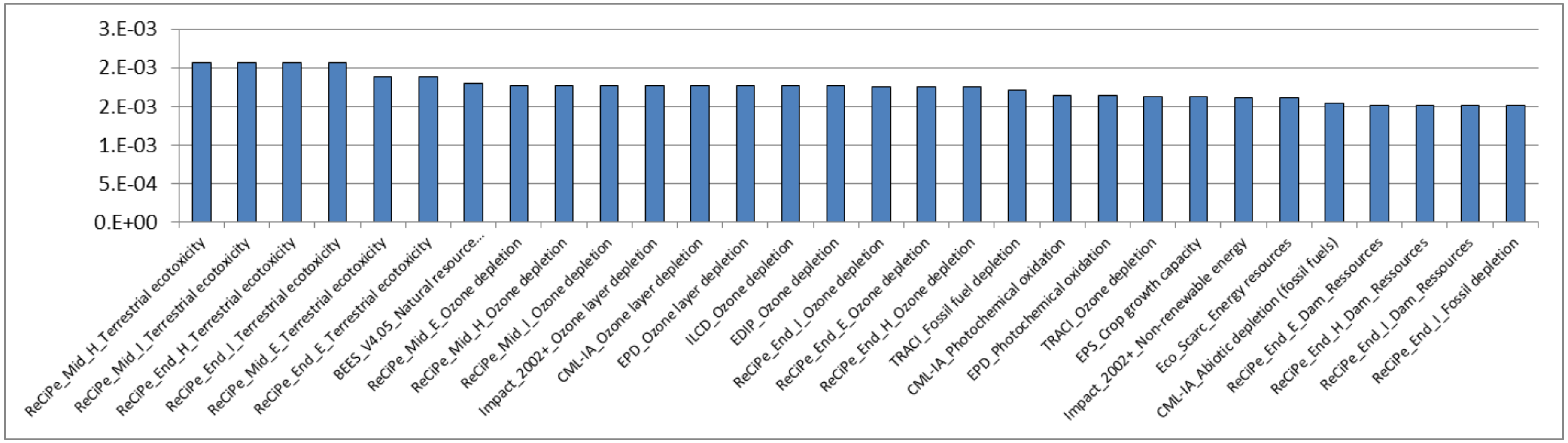


Figure S 25. Impact category RI screening for the ethanol purification step

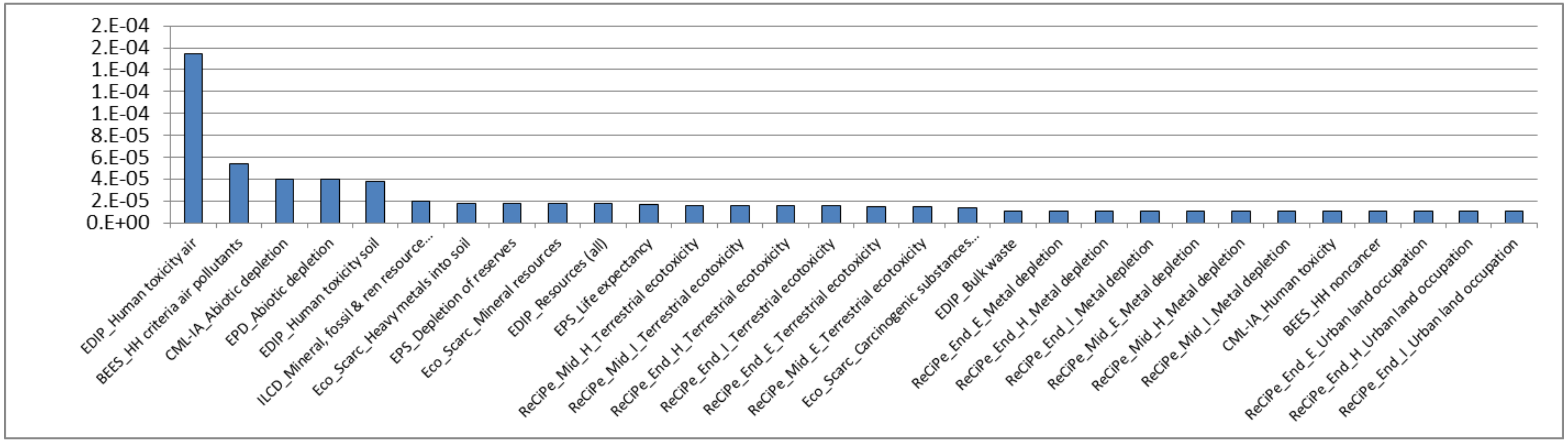


Figure S 26. Impact category RI screening for the ethanol combustion step

REPRESENTATIVENESS OF ENVIRONMENTAL ISSUES REGARDING LIFE CYCLE INVENTORY OF PRODUCTS

The Life Cycle Assessment framework (LCA) is a multi-criteria approach aiming to assess all the potential environmental impacts of any human activities. Within a standardized framework, a human activity is described throughout its values chain: from raw material extraction, through materials processing, distribution, use stages, to waste management. Then, all emission flows to the environment as well as all resource consumption flows, all defined as elementary flows, are quantified in a Life Cycle Inventory result (LCI). Translation of LCI results into a reduced number of scores that each has an environmental meaning is carried out at the Life Cycle Impact Assessment (LCIA) phase using LCIA methods. However, the holistic nature of LCA, which has induced the development of many different LCIA methods with quite a few environmental impact categories each, can make the LCIA method and impact categories selection challenging for LCA practitioners. By benefiting from a huge compilation of LCI results within cumulated LCI database, the present work develops the Representativeness Index (RI) that assesses, from a geometrical point of view, the appropriateness of LCIA methods and their impact categories for any LCI result. This innovating approach relies on the contextualization of LCI results and impact categories regarding a database and on an angular measurement within a vector space. The relevance of the RI results is tested by analysing RI trends from an entire database and by applying it to a biofuel study case.

DEFENDED ON 31/05/2018 AT : Montpellier SupAgro

WITH THE FINANCIAL SUPPORT OF : ANR elsa

INRA
SCIENCE & IMPACT

INSTITUT NATIONAL DE LA RECHERCHE AGRONOMIQUE
Unité de recherche (UR0050) - Laboratoire de Biotechnologie de l'Environnement

102, avenue des Etangs
F-11100 Narbonne
France

Tél. : + 33 4 68 42 51 51
Courriel: lbe-contact@supagro.inra.fr
www.montpellier.inra.fr/narbonne