CHALMERS
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Does my foot look big in this?

A comparison of life cycle impact assessment methods for chemical footprint calculations

Master's thesis in Industrial ecology

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Cover:
Illustration depicting the Earth, surrounded by footprints of varied sizes. Illustrated by Isabelle Asplund.

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SUMMARY

In this thesis project, eight different life cycle impact assessment methods (USEtox 2.13, EF3.1, ProScale, Environmental priority strategies, ReCiPe 2016 v1.1, Impact world +, Eco-cost and Environmental prices) for chemical footprint calculations have been categorized and evaluated based on their accessibility, ease-of-use, and characteristics. This has been done by studying literature on the chemical footprint concept and literature for each method, as well as collection of preexisting characterization factors for a set list of substances, or calculation of new characterization factors when possible. Additionally, a life cycle assessment was made for a simple production system, to test the characterization factors and increase understanding of the impact assessment methods used in a life cycle assessment. Data on physiochemical properties, fate parameters and toxicity were collected for all substances that were missing predefined characterization factors in the method USEtox 2.13 and EF3.1, as well as vapor pressure for all substances. For substances not included in the method ProScale, hazard statements were also collected.

After collecting and/or calculating characterization factors for each method, the ease-of-use of the methods was evaluated and the characterization factors for each method were compiled and analyzed. The analysis included a comparison of the substance coverages of the different methods, an evaluation of the ease-of use, a comparison of methods based the USEtox model structure, and a comparison of methods based on different model structures. The result output types were discussed as well. These comparisons were complemented by the results from the life cycle assessment.

The findings from the project are that collection of data for calculation of new characterization factors can be challenging depending on the complexity of the method, mainly linked to the parameters required. Especially the handling of toxicity data without expert knowledge in toxicology was found to be challenging. It has been possible to categorize the methods into two structural groups: multimedia fate-exposure models, with a sub-category of monetary methods, and scoring models based on hazard bandings. Finally, no method was said to be the optimal in all contexts, but what could be considered important aspects in different decision contexts was discussed.

Keywords: chemical footprint, life cycle assessment, ecotoxicity impacts, human toxicity impacts, characterization factors, life cycle impact assessment

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List of abbreviations

CF – Characterization Factor
CLP – Classification, Labelling and Packaging
CRA – Chemical Risk Assessment
CTU – Comparative Toxic Unit
DALY – Disability-Adjusted Life Years
ECHA – European Chemicals Agency
EF – Environmental Footprint
EFSA – European Food Safety Authority
ELU – Environmental Load Unit
EPS – Environmental Priority Strategies
ERC – Environmental Release Category
IARC – International Agency for Research on Cancer
JRC – Joint Research Center
LCA – Life Cycle Assessment
LCI – Life Cycle Inventory
LCIA – Life Cycle Impact Assessment
MF – Mass flow
NEX – Normalized Extinction of Species
PAF – Potentially Affected Fraction
PDF – Potentially Damaged Fraction
PHF – Person-Hour Factor
PPDB – Pesticide Properties Database
PROC – Process Category
REACH – Registration, Evaluation, and Authorization and Restriction of Chemicals
SSD – Species Sensitivity Distribution
VOC – Volatile Organic Compounds
YOLL – Years of Lost Life

1 Introduction

The introduction of new chemicals and chemical processes has been significant in the historical development of civilization (Naidu et al., 2021). For example, the invention of the Haber-Bosch process streamlined food production in the early 20th century by making synthetic fertilizers available (Tamaru, 1991). Pharmaceutical advancements are another example that has improved people's health worldwide, by the introduction of new medicines over the last century (Campos et al., 2019). This development continues today, with the chemical market being the second largest market in the world (pharmaceuticals included) (United Nations Environment Programme, 2019). The dependency on chemicals is apparent and is predicted to continue into the future as well.

Still, there is a downside to the vast use of chemicals, as large quantities of pollutants and hazardous substances are released in nature, impacting ecosystems and human health. In 2017, 62 % of the chemicals produced within the EU were considered to be hazardous to health, meaning that they have the potential to cause harm under certain circumstances (United Nations Environment Programme, 2019).

Globally, over 350 000 chemicals and chemical mixtures are registered for production and use today (Wang et al., 2020). It is therefore important that there are methods for quantifying and monitoring chemical use to safeguard a sustainable society (Diamond et al., 2015). To understand the chemical use in industrial supply chains, Fantke and Ernstoff (2018) suggest a holistic approach. By following the lifecycle of a product or a service, one could understand where in the lifecycle harmful emissions will occur, and therefore also where to focus one's efforts in order to minimize the product's, process' or service's impact.

1.1 Life cycle assessment

Life cycle assessment (LCA) is a comprehensive standardized (ISO 14040) method for assessing potential impacts associated with all phases of the lifecycle of a product or service (Technical Committee ISO/TC 207, 2006). The life cycle is usually described as "cradle-to-grave", including processes such as raw material extraction, transportation, production, use and end-of-life (Muralikrishna & Manickam, 2017). An LCA lists all the inputs and outputs in the system to cover the potential impacts. The use of "potential" is to emphasize that the quantified impact is based on a simplified model with limitations considering aspects such as time and space (Bjørn et al., 2018).

There are different kinds of LCAs, depending on what the focus of the analysis is. If environmental impacts are the main objects of the study, an environmental LCA is carried out. If social issues are of interest, a social LCA can be performed, quantifying the expected consequences on, for instance, working hours, cultural heritage or corruption (Benoît et al., 2010).

The application of an LCA can be of help with multiple issues, like for example when searching for the lifecycle of a product or service, associated with a requested function, with the least environmental impact as possible, when taking decisions regarding a strategy, product- or process design, or when making environmental declarations needed for eco-labeling or such (Jacquemin et al., 2012; Muralikrishna & Manickam, 2017).

Because of this, LCA is often used as a method for facilitating decision-making (Pryshlakivsky & Searcy, 2021).

An LCA is based on the function of the product or service analyzed, instead of its specific physical characteristics (de Simone Souza et al., 2021). For example, a floor can differ in its physical composition, hence by emphasizing the function of the floor, for example providing a durable indoor workspace, this would enable a comparison between for example wooden, carpet or tile floors. Instead of comparing 1 kg of the separate floors, 1 m^2 of floor to be used for 20 years could be compared, resulting in what is referred to as a "functional unit".

Typically, the most time-consuming step in an LCA is the collection of the life cycle inventory (LCI), which lists all the inputs and outputs (resources and emissions) from the unit processes which are the upstream and downstream processes that are needed to produce the studied product/service and is scaled by the functional unit (Saavedra-Rubio et al., 2022). To assess the potential impact from the inventory processes, the quantified resources and emissions leaving the system boundaries will be classified and categorized in the following step, the life cycle impact assessment (LCIA). LCA can include many different impact categories, including for example climate change, ozone depletion, eutrophication, and acidification (Jacquemin et al., 2012).

The translation of the inventory to impacts is conducted through multiplication of flows with characterization factors (CFs) for the chosen impact categories. The CFs harmonize the impacts within a certain impact category to be evaluated on a common basis, enabling impacts from different substances to be added into a joint potential impact for that category. There are two different levels for CFs: midpoint and endpoint level, differing in the presentation of the impact results. The midpoint CFs translates the LCI flows into potential effects of emissions and resource acquisitions based on cause-effect chain modelling and quantifying an effect that is not at the very end of the cause-effect chain of events. For example, climate change effects are often quantified as emissions of carbon dioxide equivalents, meaning the potential to influence radiative forcing. The endpoint CFs translates the LCI flows into indicators for areas of protection (i.e. ecosystems, human health, resource availability), resulting in a wider grouping (Sala et al., 2012).

Together, LCI and LCIA give a potential impact of the product or service studied, making up the full LCA results which in a last step can be interpreted and used for decision making, e.g. selecting a material, process solution or product. An LCA can further include steps such as weighting and normalization, with the aim of comparing different impact categories.

1.2 Chemical footprint

The assessment of ecotoxicity and human toxicity (hereinafter (eco)toxicity) impacts can vary between different LCIA methods and can include different impact categories based on their scopes and approaches (Frontera et al., 2020). The toxicity impact categories are often divided into human- and ecotoxicity, where the human toxicity category is often further divided into cancer and non-cancer effects.

For the (eco)toxicity impact categories the potential impact can be called the "chemical footprint" of a product, similar to the standardized and more commonly known concept

of “carbon footprint”, which aggregates the amount of greenhouse gases (represented by carbon dioxide equivalents) released by a product or service during its lifecycle (Wiedmann & Minx, 2008). The chemical footprint concept is not as established as the carbon footprint; hence several definitions can be found in literature (Rydberg et al., 2014). Most definitions include lifecycle thinking, chemical, hazard and exposure assessment and sustainability assessment to various extents. The sustainability assessment includes referring the obtained toxicity value to a threshold, like a set carrying capacity for an ecosystem or a safe exposure limit. For this report, the chemical footprint will be defined as the aggregated potential (eco)toxicity impact of all substances emitted during the lifecycle of a product, process or service, disregarding a further sustainability assessment. This definition is based on literature regarding the concept of chemical footprint (Hitchcock et al., 2012; Sala & Goralczyk, 2013).

Chemical footprint assessment is often based on the principles of chemical risk assessment, CRA. This involves considering aspects such as exposure, fate and effect (Margni et al., 2002). Fate processes are dependent on the movement the substance will have in different compartments, such as soil, air, or water. This considers, for example, advection, volatilization, and sedimentation. It also involves the process of degradation. The concept of exposure refers to the intake routes from the substances to the receptor (human, animal, or ecosystem). An exposure can be direct, like in industrial settings where a worker is in direct contact with a chemical, or indirect, whereas the substance travels via the environment, involving processes like bioaccumulation where the chemical has moved through different organisms and compartments before the receptor is exposed to it, e.g., via food, feed, air, and water. Finally, the exposure of the substance is compared with an effect level, which is the level that an adverse effect has been detected. This level is usually found through laboratory testing on animals or cells.

The combination of fate, exposure and effect constitutes the foundation for the CF calculations, although different parameters can be used in different LCIA methods. The calculation of CFs enables a comparison between the impact of the substances to assess the potential impacts from the product system on ecosystems and human health, resulting in a chemical footprint.

1.2.1 Life cycle impact assessment methods for (eco)toxicity

It is a challenge to conduct a chemical footprint, considering the multiple previously mentioned aspects (Gust et al., 2016). There are therefore a few methods in use today and they differ in scope and model structure.

USEtox is an LCIA method developed in 2008 by the United Nations Environmental Programme – Society of Environmental Toxicology and Chemistry (UNEP-SETAC) aiming to establish a consensus method, based on previous toxicity LCIA methods (Westh et al., 2015). The method can be found as fully implemented in various LCA models, or it can be used separately, when only assessing (eco)toxicity. There are also some LCA models that have USEtox as their basis for LCIA calculations, but with some alterations (which will later be described), such as EF3.1 (Saouter et al., 2018), Impact world + (Bulle et al., 2019), ReCiPe 2016 v1.1 (Huijbregts et al., 2017), Eco-cost (Sustainability Impact Metrics, n.d.), and Environmental prices (de Bruyn et al., 2018).

There are also methods that have a different scope than USEtox, such as ProScale (Lexén et al., 2021), that assess direct exposure and Environmental Priority Strategies (EPS) (Steen, 1999), that are a method based on empirical data, both methods will be further addressed in this report.

1.3 Project setting

The thesis has been part of the project: User friendly tools for industry to measure and reduce chemical footprints (Tox-redUSE) at IVL Swedish Environmental Research Institute (hereafter referred to as IVL). The project aims to lower the threshold for implementing chemical footprint calculations within an industrial setting. The project idea is that for companies to report on and try to minimize their chemical footprint, the tools for calculating the impact must be user-friendly, while still delivering results that can be used in a decision-making process.

1.4 Aim

The aim of the thesis project has been to evaluate a selected number of LCIA methods for calculating a chemical footprint regarding their useability for industry actors. By using the different methods, CFs have been calculated for a wide range of substances with different chemical properties. Following that, the methods were evaluated based on the relevance of the results (depending on decision context), how easy the methods were to use and what was needed to use them in a correct way. The performed mapping of the LCIA methods should later act as a support for industrial users when deciding on which method to use for measuring chemical footprints, obtaining results that can act as a foundation for decisions in contexts such as innovation, purchase, and communication.

1.5 Limitations

The thesis relied on literature, data from public/licensed (where applicable) databases and on calculations based on this literature and data. In case of missing data for any chemical, predictive methods were used to fill the gaps.

While the prioritizing of methods and substances aimed at covering a wide span of scenarios, this also limited the extensiveness of the study. The study covered a selection of LCIA methods for calculating characterization factors. The starting point was an initial mapping of LCIA methods that was made for the Tox-redUSE project (Andersson et al., 2024). Only open-access methods and methods for which IVL has a license were included.

Also, a decided set of substances was considered, aiming to cover a broad range of chemical properties. The initial substance list was also given by IVL.

Access to confidential data given during the course of the project was treated as confidential and returned to IVL after the project ends. No confidential information is included in this final public report.

1.6 Specification of the issue being investigated

To reach the aim of the thesis, answers have been searched for the following research questions:

- How can the methods to calculate chemical footprints be categorized based on their accessibility and ease-of-use?
    - This includes a structured assessment of how complex the method is, how easy it is to get access to its input data and the correct use of the results.
- What characterizes the different methods to calculate chemical footprint?
    - This includes a comparative description of model structure and the resulting characterization factors for the substance list under study.
- Can recommendations be given on what method to calculate chemical footprint that is suitable for a given decision context?
    - Examples of decision contexts are innovation, purchase, and communication, but consideration needs also to be made on system specific characteristics, e.g., on the type of material and/or substance.

2 Method

The thesis work was divided into different tasks. A literature reviewing process was carried out throughout the project, with the initial focus of gathering background information for prioritizing the LCIA methods and later focusing on more in-depth information gathering for further understanding of the selected methods. Additionally, a systematic literature review of the chemical footprint concept was made, which can be found in section 2.1 below. For the substances under study, an initial substance list proposal was provided by IVL, and then complemented with additional substances of interest. With the substance list in place and a prioritization order of methods set, a data collection process was initiated, collecting physiochemical data, fate parameters and toxicity data for substances which were missing CFs in the methods for which calculation of new CFs were possible. After finalizing the data collection, CFs were gathered and, if possible, calculated. When CFs for all the LCIA methods were acquired, a comparison of characterization results within and between methods could be made. The user experiences from the different methods were also evaluated. Finally, an LCA for a small production system was made, using the CFs from the different methods to assess the chemical footprint of the system. It was then possible to analyse how the result of the LCA changed based on which method was used.

2.1 Literature review

A continuous search for literature was performed throughout the whole period of the project. The focus of this continuous literature study was to understand why there are different LCIA methods for chemical footprint calculations, how they relate to each other and how they are used. The literature was found partly through use of the scientific search engines Scopus and Google Scholar, and partly through use of the sources from the initial mapping report for the project Tox-redUSE given by IVL (Andersson et al., 2024). Phrases and words used for finding articles in the databases were “life cycle assessment”, “LCA” and “life cycle impact assessment” in combination with “toxicity”, “chemical footprint” and “decision-making”.

For background information on the LCIA methods and their use, literature regarding each method was consulted. First, the manuals for the methods were studied, if available. Following that, scientific articles about the background and structure of the methods were read, which was later completed with additional literature on updates of the methods, comparisons with other methods and case-study examples if judged to be of help for the understanding of the method. Some of this literature was sourced from the Tox-redUSE mapping report (Andersson et al., 2024), in which the main documents for each method studied were referenced.

In addition, a systematic literature review was made for the concept of the chemical footprint. When searched for in Scopus, the input “chemical footprint” (also the variations of “chemical footprints” and “chemical-footprint") was included in the title, abstract or as a keyword for 176 documents. Out of those documents, seven were written in a language other than English and therefore disregarded. Since several documents related to

chemical footprint in the context of DNA footprinting[1] instead of the toxicity impact assessment method of interest, additional tapering was made. To avoid results focusing on other contexts than the intended, the following subject areas were excluded from the search: dentistry, economics, econometrics and finance, immunology and microbiology, computer science, medicine, neuroscience, pharmacology, toxicology and pharmaceutics, physics and astronomy, biochemistry, genetics and molecular biology, agricultural and biological sciences, and energy. Adding this filter, 70 documents remained.

The titles and abstracts of the 70 documents were inspected to find the texts that defined, discussed, or evaluated chemical footprint as a concept. Several results described the use of the chemical footprint concept in different case studies but did not contribute further into a conceptual understanding or definition. After selection, 12 articles were kept for further understanding of the chemical footprint concept and its definitions. Two additional articles were added to the review of the concept, sourced from the Tox-redUSE mapping report, resulting in a total number of 14 articles to be studied. The two additional articles that were added were not captured in the Scopus search since one of them focused on environmental footprints as concept and not specifically on chemical footprints, while the other one was not available through Scopus. All studied articles are listed in Table 8 Appendix A.

The 14 articles were analysed based on five aspects: how the chemical footprint was defined and structured, whether it took any geographic boundaries into consideration, if the chemical footprint was said to have a specific unit, and if the footprint was described as pressure or impact driven.

The findings from the literature study are presented in section 3.1.

2.2 Selection of LCIA methods and substances

To ensure that the project covered a broad range of LCIA methods and substances a careful selection of both were made. The LCIA methods were put into groups of high, intermediate, and low priority based on criteria described in the section below.

2.2.1 LCIA methods

Initially, a list of LCIA methods was taken from the mapping report for the project Tox-redUSE at IVL (Andersson et al., 2024). This list concluded 16 different LCIA methods. Priority was given to methods that differed in origins and structures, to ensure that a variation of methods would be tested. Models from three structural categories were studied: multimedia fate-exposure models, scoring models based on hazard banding and monetary methods.

The methods were put into groups of high, intermediate, or low priority based on aspects covered in Table 1. The assessment followed the priority order presented in the table. Initially, six methods were put into the intermediate priority category but out of those only four were assessed. The remaining three methods were disregarded based on them

[1] DNA footprinting refers to methods used for analysis of protein-DNA complexes and identification of binding site positions on a DNA sequence. Rojo, F. (2013). DNA Footprinting. In S. Maloy & K. Hughes (Eds.), *Brenner's Encyclopedia of Genetics (Second Edition)* (pp. 360-363). Academic Press. https://doi.org/https://doi.org/10.1016/B978-0-12-374984-0.00420-4

not covering toxicity impacts, not being able to access or too much overlap with the highly prioritized methods. The methods that were assigned low priority were also disregarded. The final list of assessed LCIA methods is presented in Table 1.

Table 1. Basis for order of priority for the LCIA methods. O = organic substances, I = inorganic substances, M = metals, HT = human toxicity, ET = ecotoxicity. *No model template of its own, but possible to make described adjustments to USEtox 2.1.

LCIA method	Substance coverage	Toxicity coverage	Structural category	CF calcul-ations possible	Reference	Priority
USEtox 2.13	O, M	HT, ET	Multimedia	Yes	(Rosenbaum et al., 2008)	High
ProScale-H	O, I, M	HT	Hazard banding	Yes	(Lexén et al., 2021)	High
Environmental Footprint 3.1	O, I, M	HT, ET	Multimedia	Yes*	(Saouter et al., 2018)	High
Environmen Tal Priority Strategies, EPS	O, I, M	HT, ET	Monetary	No	(Steen, 1999)	High
Eco-cost	O, M	HT, ET	Monetary	No	(Sustainability Impact Metrics, n.d.)	Intermediate
Environmental prices	O, M	HT, ET	Monetary	No	(de Bruyn et al., 2018)	Intermediate
Impact world +	O, M	HT, ET	Multimedia	No	(Bulle et al., 2019)	Intermediate
ReCiPe 2016 v1.1	O, M	HT, ET	Multimedia	No	(Huijbregts et al., 2017)	Intermediate

2.2.2 Substances

The substances included were chosen to represent varying properties and structures within the substance classes organic and inorganic substances (including metals). The starting point was inventories of substances expected to be emitted in the manufacture of selected industry chemicals, i.e., relevant representation of substances that must be characterized for the calculation of a chemical footprint for that specific industry chemical. To ensure wide coverage of substance classes and properties directed additions was made to the inventory-based list.

The final substance list included a selection of substances from the inventory of two plasticisers: di-2-ethylhexyl phthalate (DEHP) and epoxidized soybean oil (ESBO) (Caldeira et al., 2023), four pesticides: cyfluthrin, glyphosate, glutaraldehyde and 2-methyl-4-chlorophenoxyacetic acid, (MCPA), six other substances of high concern: perfluorooctanesulfonic acid (PFOS), perfluorooctanoic acid (PFOA), 8:2 fluorotelomer alcohol (8:2 FTOH), atrazine, methylisothiazolinone (MIT), and benzoethiazole, and then

the three substances with the highest midpoint characterization factor for the categories ecotoxicity, human toxicity – cancer and human toxicity - non-cancer, respectively, in USEtox 2.13 (Rosenbaum et al., 2008). These substances are indicated with an asterisk (*) in Table 9 in Appendix A. For the ecotoxicity category, the substances were chosen based on the characterization factor for the freshwater compartment, while for the two human toxicity categories, the substances were selected based on the emission to household indoor air.

In order to evaluate how well the methods handle a dissociating substance, and also cover a pure metal, the two components of aluminium sulphate when dissociated (aluminium and sulphate) were also included.

In total, this compiled into a list of 73 substances. The complete list can be found in Table 9 in Appendix A.

2.3 Data collection strategy

Calculations of new CFs were made for the substances missing predefined CFs, for the methods in which calculations were possible. This required data on physio-chemical properties and fate parameters, (eco)toxicity data, and hazard statements. Full sets of data were only collected for the substances without CFs in USEtox 2.13 and/or EF3.1. Additionally, vapor pressure data were also collected for all fluid substances, to be used in ProScale. All data were collected from open, online databases, listed below.

To ensure a systematic collection of data, the data sources were ranked in order of preference. The two different priority orders were used, depending on if data were collected for USEtox 2.13 and ProScale or for EF3.1. The data base priority order for USEtox 2.13 and ProScale was as follows:

1. CompTox (United States Environmental Protection Agency, 2021)
2. European Chemicals Agency, ECHA/REACH (European Chemicals Agency, n.d.)
3. PubChem (National Library of Medicine, n.d.)
4. EPIsuite (United States Environmental Protection Agency, 2012)

CompTox was selected as the first-hand database to consider when searching for data. This was because it provided an easy overview of the physio-chemical properties needed, and it was possible to collect toxicity test data in batch, which was considered important to efficiently collect data for the number of substances handled in the project. In CompTox, data from different sources is compiled. This means that data collected from CompTox may originate from one of the lower ranked data bases, often ECHA or EPIsuite.

ECHA/REACH was included since it contains data reported from companies within the EU and is one of the recommended data bases for use in EF3.1 (Saouter et al., 2018). ECHA was listed as the second data base to consult based on this, as well as that the website was easy to navigate, containing multiple different substance properties and fate parameters.

As a third alternative, PubChem was used. PubChem also contained a compilation of data from other sources, often covering several physiochemical properties and fate parameters. However, data are sometimes given in a body of text, making them difficult

to collect. Because of this, PubChem was ranked as the third data base option data collection.

The last option for the data collection was to use EPIsuite to estimate substance properties and fate parameters. Since the use of estimated data introduces uncertainties to the results, this option was the least preferred, but used when filling of data gaps was needed.

The EF3.1 method prioritizes use of European data. Because of this, for the calculations of CFs using EF3.1, an alternative data base priority order was used:

1. European Chemicals Agency, ECHA/REACH (European Chemicals Agency, n.d.)
2. CompTox (United States Environmental Protection Agency, 2021)
3. PubChem (National Library of Medicine, n.d.)
4. EPIsuite (United States Environmental Protection Agency, 2012)

Data from ECHA/REACH were prioritized to collect data in line with the instructions for the EF3.1 method (Saouter et al., 2018). However, if data from this database could not fill all parameters, CompTox, PubChem and EPIsuite were used to fill those gaps, disregarding the database preference in EF3.1.

2.3.1 Physio-chemical properties and fate parameter collection

To minimize the time spent working on data and data collection, only the first value found for a certain characteristic was collected for the physio-chemical properties and fate parameters.

When collecting physio-chemical data, experimental data were preferred to estimated data. If presented with both average and median data options, median values were preferred since they should be less impacted by any potential outliers (data points that deviate from the trend) than a mean value would. If faced with data gaps, EPIsuite was used to predict data. For some substances, EPIsuite presented experimental values that were logged in the program. In those cases, like for all other data collection points, the experimental values were preferred to the predicted values. The EPIsuite program was used to cover data gaps for all kinds of substances, no matter substance groups (organic/inorganic/metals). However, inorganic compounds are outside the estimation domain of EPIsuite which affects the reliability of the predictions for those substances. Inorganic compounds are presented separately in the result to ensure that they can be studied independently from the organic substances which have been calculated for within the domain of use for EPIsuite, when used.

2.3.1.1 Dustiness parameter in ProScale

For solid substances in ProScale, a categorization of the dustiness of the substance was needed. No detailed instructions for how to assess this substance property were given in the manual (Lexén et al., 2021), only an example list of the dustiness of some materials and which category (low, medium, or high) they belong in. The substances under study for this report were compared and assessed with the example materials, and then categorized based on the aspects listed in Table 2.

Table 2. Dustiness categorization based on substance property descriptions.

Dustiness category	Substance property descriptions
Low	• Salts, as they were expected to aggregate into bigger crystals when reacting with the water in the air • Substances specified as crystalline
Medium	• Substances specified as powders
High	• Substances specified as milled or spray powders • If insufficient information is available to warrant another classification, as a worst-case scenario alternative

2.3.2 Toxicity data collection and harmonization

The toxicity data were used to calculate CFs in USEtox 2.13 (Rosenbaum et al., 2008) and EF3.1 (Saouter et al., 2018). The toxicity data was collected solely from the Toxicity Value Database (ToxValDB v9.4) in CompTox (United States Environmental Protection Agency, 2021), which consists of data sourced from multiple other databases, public datasets, and open literature. All available information about the toxicity data was collected for both human toxicity and ecotoxicity.

Toxicity data were used in USEtox 2.13 to calculate inhalation and ingestion ED50 values for human toxicity and avlogEC50 values for ecotoxicity. Before use, the data was harmonised according to Table 11 in Appendix A.

Furthermore, for carcinogenic toxicity data points, a comparison was made between the data found in the registration dossiers on the ECHA website, genotoxicity data on the Comptox Dashboard and the International agency for research on cancer (IARC) (European Chemicals Agency, n.d.), (United States Environmental Protection Agency, 2021), (IARC, n.d.). If the substance was, or had potential to be carcinogenic considering the classification in IARC, toxicity data were gathered if available from ECHA or CompTox. If no data were available, the cancerogenic ED_{50} values for the substance were left blank, indicating a data gap. If none of the websites indicated a risk for carcinogenicity, a value of zero was applied to the cancerogenic ED_{50} parameters.

2.4 Calculations and assumptions for the LCIA methods

The methods had precalculated CFs for most of the substances in the substance list available. However, when a substance was missing a CF, calculations were made when instructions/software was available. The calculations required different data depending on the method. This did sometimes require unit conversions and extrapolations, for example, approximation of chronic effects from acute effect data by use of a factor. Additional calculations to what was written in the manuals or programmed in the software, respectively, and assumptions, are presented in this section.

2.4.1 Calculation procesdure in USEtox 2.13

Calculations of CFs missing in USEtox 2.13 were possible using the downloadable USEtox tool (MS Excel sheet) (Rosenbaum et al., 2008). Several physio-chemical properties and toxicity data points were fed into the software, which could then be run, giving CFs for (eco)toxicity on both mid- and endpoint level. Calculations were made in the same way for organic and inorganic substances (not including metals), following the calculation process described for organic substances and departing from the described calculation process specifically intended for inorganic substances in the USEtox 2.0 manual (Fantke et al., 2015c)**.** This was because the data needed for the intended process for calculations of inorganic substances were difficult to obtain, so in order to get any CFs for inorganic substances at all, this approach was implemented. However, it should be noted that the CFs resulting from this practice should be viewed with caution and be seen more as an experiment to assess the calculation process in USEtox 2.13.

Due to a lack of instructions in the USEtox 2.0 manual (Fantke et al., 2015c), some additional calculations were made, listed in Table 3.

Table 3. Conversions made to the toxicity data used in USEtox 2.13. HT = human toxicity, ET = ecotoxicity.

Conversion	**Toxicity type**	**Missing instruction**	**Calculation pathway**	**Reference**
NOAEC to ED_{50}	HT	No instructions in the manual for how to handle NOAEC-data, which cannot be handled by the software in its calculation sheet "Human tox ED50".	NOAEC-data were converted into ED_{50}-data by: 1. Multiplication of 9, resulting in an EC_{50} value. 2. Applying the EC_{50} value in the USEtox 2.13 tool converting it into a ED_{50} value.	Species extrapolation factor for inhalation of 1 and conversion from NOAEC to EC_{50}: (Fantke et al., 2015c)
ppm to mg/m3	HT, ET	No instructions for how to handle other units than mg/m3 for inhalative tests.	Concentration in ppm was converted to mg/m3 through multiplication of the concentration in ppm with 0.0409 and the molecular weight of the substance under study.	(Boguski, 2006)
NOEL to EC_{50}	ET	No instructions for how to handle other points of departure than chronic and	Chronic NOEC-data were converted into chronic EC50-data by division with 0.4. Acute NOEC-data were converted into	(Aurisano et al., 2019)

		acute EC_{50} values in the software in its calculation sheet "avlogEC50".	chronic EC_{50}-data by division with 1.2.	

Following the USEtox 2.0 manual for organic substances (Fantke et al., 2015d), it was possible to calculate degradation factors for soil and sediment based on the degradation in water by applying conversion factors for those. The degradation rate in air could be calculated using the hydroxyl radical rate for the substances when available, also according to the USEtox 2.0 manual for organic substances.

Furthermore, since degradation factors in water were missing for aluminum sulphate, calcium chloride and sodium silicate, the assumptions were made that the degradation for those substances could be set equal to other similar substances (salts). These substances are assumed to dissociate into its ion constituents when dissolved in water. When dissociated, the dissolved ions will act differently than their solid, neutral equivalents, which are modelled in USEtox. The ionization take place in water, affecting the transport processes in all environmental compartments. Neither inorganic (other than cationic metals) nor dissociating substances are within the scope of USEtox. To consider the dissociation into ions the substances could instead be modelled as their ion constituents.

2.4.2 Calculation procedure for Environmental footprint 3.1

Calculations of CFs missing in EF3.1 were conducted by making adjustments in the USEtox 2.1 model (Rosenbaum et al., 2008) according to the manual by (Saouter et al., 2018). The EF method prioritizes use of European data from ECHA-REACH, EFSA and PPDB. However, to streamline the data collection process, this was not followed entirely. Instead, physiochemical data and fate parameters were collected according to the data collection strategy presented in section 2.3.1

The toxicity data were also collected according to section 2.3.2, coming from CompTox (United States Environmental Protection Agency, 2021). CompTox did however include data from the European database ECHA IUCLID, which was the source for most human toxicological data. For the ecotoxicological data, most of it originated from ECOTOX, which is a toxicology database from the United States Environmental Protection Agency.

EF3.1 required ecotoxicological data to be converted into a HC_{20} value, instead of a HC_{50} (same as $avlog_{EC50}$) value as in USEtox. The manual instructs the analyst to get the HC_{20} value by creating a species sensitivity distribution (SSD) curve using the collected toxicity test data. Herein, a simplified approach was used instead. If only one species toxicity value is available, the manual described how to go from a HC_{50} value to a HC_{20} value using extrapolation factors adapted for different substance groups, like organics, inorganics, elements, and petroleum products. This approach was used to extrapolate HC_{20} values for all substances missing CFs in EF3.1 from HC_{50} values calculated for use for calculating CFs in USEtox 2.13 (Rosenbaum et al., 2008).

The mentioned adjustments were added to the USEtox 2.13 template and run, giving approximate CFs for EF3.1 (due to deviations in data collection and USEtox model version the resulting CFs will not be identical to CFs if the same substances would be included in the EF3.1 CF tables). It should be noted that EF3.1 is based on USEtox version 2.1, not version 2.13 which was used for this study.

The emission compartments used in EF3.1 and in USEtox 2.1 differ slightly, hence, some alterations had to be made after obtaining the CFs from USEtox. For example, emissions to air, indoor in EF3.1 are equivalent to the average of the emission compartments household and industrial indoor air in USEtox 2.1 (Saouter et al., 2018) (Table 48 in that report).

The midpoint CFs that were achieved were converted into endpoint CFs in order to be comparable with the results of other methods. For this conversion, the same midpoint-to-endpoint conversion factor as in USEtox was used, hence the midpoint CFs for human toxicity were multiplied with 11.5 for cancer effects and 2.7 for non-cancer effects to get to DALY (Fantke et al., 2017). For ecotoxicity, the same approach was used, but the midpoint CFs were multiplied with 0.5 to go from PAF to PDF (Fantke et al., 2017).

2.4.3 Calculation procedure for ProScale

The calculations of CFs in ProScale were made using the ProScale Excel tool version 1.6 (available through the ProScale technical secretariat, Tomas Rydberg, IVL). For the substances missing H-phrases, they were added manually in the sheet "H-Phrase-Database". The missing H-phrases were collected according to the data hierarchy presented earlier, in section 2.3, in which CompTox presented hazard statements retrieved from the ECHA website. This is also in line with the described data collection hierarchy described in the ProScale manual (Lexén et al., 2021). Only hazard statements with more than 10% of classifications identified by the registrations were used.

As ProScale combined inventory modelling and impact assessment, a default person-hour factor (PHF) and process category (PROC) were assigned to arrive at a score representative of a CF. The mass flow (MF) was consistently set to 1. The PHF was set to 0.003 h/kg substance, a default value for a manufacturing processes in organic commodity chemicals manufacturing, in a small to medium size chemical plant, obtained from the ProScale manual (Lexén et al., 2021). The PROC chosen was number 4: chemical production where opportunity for exposure arises. This was to ensure that substance properties affecting exposure would be reflected in the score. The type of setting was set to "industrial".

Additionally, the state of each substance (fluid/solid) was filled in together with the vapor pressure, if a fluid, and the dustiness, if a solid. Vapor pressure data were collected according to the physio-chemical property data collection described in section Physio-chemical properties and fate parameter collection, and the dustiness was assessed according to section 2.3.1.1 in this thesis.

No local exhaust ventilation, respiratory protection or dermal personal protective equipment was included.

2.4.4 Calculation procedure for Environmental priority strategies

No additional CFs were calculated in Environmental priority strategies (EPS). CFs for (eco)toxicity were found in the substance classes volatile organic compound, VOC, and pesticides. The human health CFs were collected as an endpoint expressed in years of lost life (YOLL), with the pathways cancer and acute toxicity. The ecosystem CFs were collected as an endpoint expressed in Normalized extinction of species (NEX), referring to extinction of species during one year on a global basis.

2.4.5 Calculation procedure for the other USEtox-based methods

For the remaining LCIA methods studied, Eco-cost, Environmental prices, Impact world + and ReCiPe 2016 v1.1, the CFs were collected from their respective template or tool. No new CFs were calculated since it was not considered possible.

Egalitarian CFs were collected from ReCiPe, as it was considered a worst-case scenario, in comparison with individualist and hierarchist perspective. Environmental prices were calculated from the ReCiPe CFs, multiplying the CFs with a factor of 0.158 euro per 1.4 DCB-equivalents according to the manual (de Bruyn et al., 2018).

2.4.6 Normalization of results

The resulting CFs were normalized to selected substances to be able to compare the magnitudes of the CFs between methods with different units. It was not possible to use the same normalization substance for all toxicity categories and model comparisons since the substance coverage varied. The normalization substances were selected based on what substance that was available for all methods in the toxicity category under study. The other substances were then normalized to the selected one by dividing their CFs on the CF for the selected substance.

2.5 Data uncertainties

Deviations in data collection strategy or data handling from the procedure described in the manuals of the methods result in CFs that are highly uncertain. This can include data collected from another database than what is intended to be used, extrapolation of data using extrapolation factors or inconsistent selection of toxicity data. In order to highlight these uncertain CFs, all of the manually calculated CFs have been indicated in the result section.

For USEtox 2.13, there are also different data scenarios described in the USEtox 2.0 manual (Fantke et al., 2015c) which are said to result in less reliable CFs, in the USEtox database classified as “indicative” (Rosenbaum et al., 2008). Such scenarios are for example when the substance is out of the scope of the USEtox model (i.e. inorganic or metal), when route-to-route extrapolation is applied for human toxicological effects, or when effect factors for ecotoxicological effect factors are based on less than three trophic levels. The collected CFs that have been classified as indicative in the USEtox 2.13 database (Rosenbaum et al., 2008) are specified in Table 9 in Appendix A.

2.6 Analysis strategy

With the results in place, a structured analysis of the results was conducted to compare the methods.

The analysis included the following parts:

- Comparison of the substance coverages of the different methods.
    - This included how many substances from the substance list that had CFs included for each method, and how many CFs that were calculated, for the methods for which this was possible.
- Evaluation of ease-of-use of the different methods.
    - This evaluation was based on if there was a step-by-step guidance and how easy it was to follow.
    - The evaluation was based on the knowledge level of engineering students in their final year.
- Comparison of similar methods, based on the USEtox model structure.
    - This included an analysis of the required parameters for the organic substances with the seven highest CFs in the human toxicity and ecotoxicity categories to identify any tendencies between parameter size and toxicity potential.
    - Further distinctions between model structures were also made.
- Comparison of methods with different model structures.
- Analysis of the impact of presenting the CFs at midpoint/endpoint level.
- Comparison of methods based on a monetary approach.
- Analysis of uncertainties with the results
- Analysis of the LCA results

2.7 Life cycle assessment

To test the collected CFs and understand the LCIA methods in an LCA context, an LCA was performed. A simple system for the production of polyvinyl chloride, PVC, sheets used for flooring was modelled in the LCA software LCA for Experts (Sphera, 2024). The system was defined to include PVC granulates mixed with the plasticizer DEHP - for which the components of its formulation had been included in the substance list for the project - to produce PVC sheets. The productions of DEHP, 2-ethylhexanol and phthalic anhydride were also modelled.

The LCA methodology followed was based on the ISO14040 standard but did not follow the standard in full.

2.7.1 Goal and scope definition

The potential environmental impact was assessed, focusing on (eco)toxicity, for the cradle-to-gate process of the production of PVC sheets used for flooring. This was a curiosity-driven LCA for which the goal was to learn about LCIA methods, test calculation outcomes and the feasibility of chemical footprint methods, Hence, the functional unit is defined as 1 m^2 PVC floor used in a public building for 20 years, which corresponds to a mass of 2.5 kg for public PVC flooring (Baitz et al., 2004). The system is defined to take place within a European setting, having the manufacture of DEHP take place in Germany and of PVC granulates in Belgium. These components were then assumed to be transported to Sweden, for the final production of PVC sheets.

Different LCIA methods were tested to evaluate the difference in their toxicity assessment. Manually calculated CFs were also inserted into the LCA software, to evaluate the size of the impact that such calculated CFs could have.

When modelling the system in GaBi, formaldehyde was used as proxy for butyraldehyde since butyraldehyde was missing in the database and formaldehyde was assumed to be a similar substance with similar toxic impacts. However, it was later discovered that the upstream productions of the two substances differed greatly, so the use of formaldehyde as a proxy for butyraldehyde was not ideal or as representative as hoped for. But, since the LCA was performed mainly to test out the CFs and get a deepened understanding of the impact of using different LCIA methods, this mistake was accepted and used anyway.

2.7.2 Life cycle inventory

Data were collected mainly on the substances used in the process, for which predefined processes were missing in LCA for Experts. The composition and inventory of PVC sheets used for flooring was retrieved from Baitz et al. (2004). For the production processes of DEHP, 2-ethylhexanol and phthalic anhydride, the composition and inventory were given by Caldeira et al. (2023) and T. Kärnman (personal communication, April 29th and May 7th, 2024), and modelled as described by T. Kärnman (personal communication, April 29th and May 7th, 2024). The four foreground processes (production of 2-ethylhexanol, phthalic anhydride, DEHP and PVC sheets) were assigned different environmental release categories, ERCs, based on their characteristics. The first three manufacturing processes were assigned ERC 1, for manufacture of substances, and the PVC sheet production was assigned ERC 3, for formulation in materials (ECHA, 2009). The default worst-case release factors for ERC 1 were 5% to air, 6% to water and 0.01% to soil (ECHA, 2016). For ERC 3, the corresponding factors were 30%, 0.2% and 0.1% for the air, water, and soil compartments, respectively.

The processes which were already available in LCA for Experts were used when possible. These were aggregated processes, meaning they included upstream process steps and their coupled in- and outflows.

The modelled system is shown in the flowchart in Figure 1.

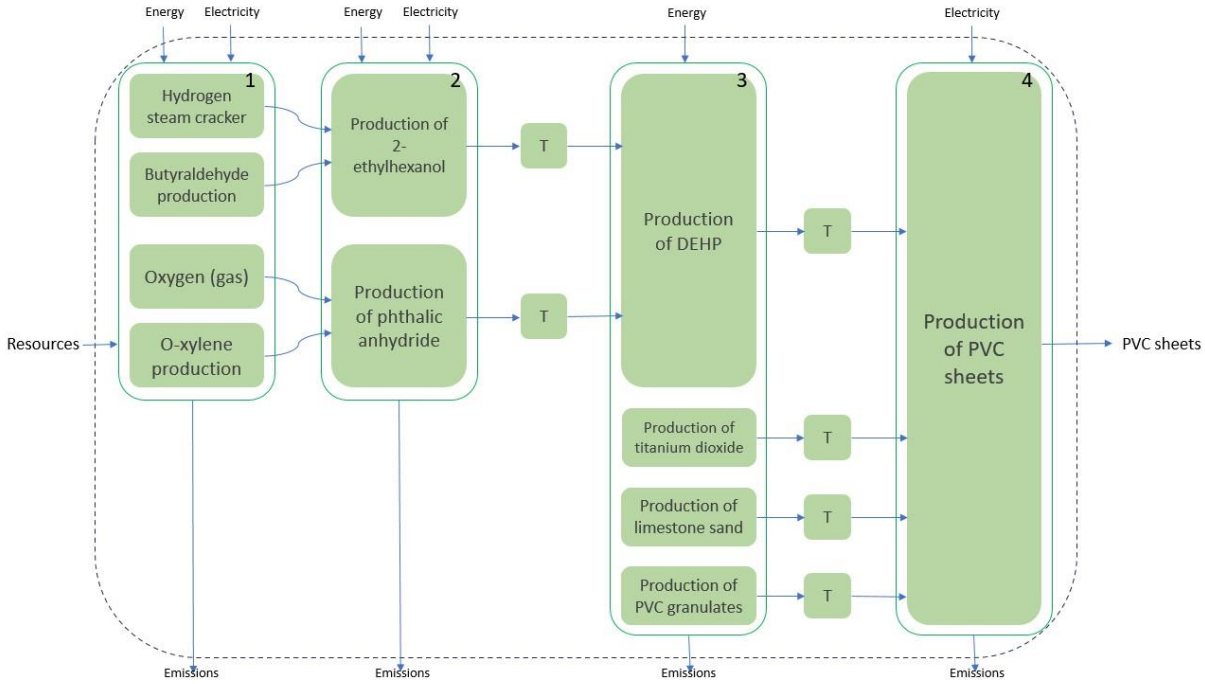

Figure 1. Flowchart of a simple system for production of PVC sheets used for flooring.

The inventory of the PVC flooring production modelled is presented in Table 12-Table 17, found in Appendix B.

2.7.3 Life cycle impact assessment

The inventory data were classified and characterized by the impact assessment methods EF3.1, ReCiPe 2016 v1.1 (E), USEtox 2.12 and USEtox 2.12 with added CFs from calculations made in this project. These methods were used since they were already included in LCA for Experts. The EPS method was also available in the software but was not used since the possibilities to extract only toxicity impacts were limited.

For the four non-adjusted methods, imbedded CFs were used and for the substance emissions with missing CFs - no CFs were added. For the adjusted USEtox 2.12 version in which calculated CFs from this project were used, CFs were added for the following substances: ammonia (CAS: 7664-41-7), chlorine (7782-50-5), hydrogen fluoride (CAS: 7664-39-3), hydrogen peroxide (CAS: 7722-84-1), sodium sulphate (CAS: 7757-82-6).

The processes in the PVC production process chain were grouped based on their place in the production chain. For example, processes supplying the production of 2-ethyhexanol, and phthalic anhydride were put into group one. 2-ethylhexanol and phthalic anhydride were in turn put into group two, as suppliers to the production of DEHP, and so on, leading up to the PVC production being the fourth, last group. Additionally, the transport processes and energy processes were grouped.

The methods were analyzed based on the impact categories of ecotoxicity, human toxicity cancer and non-cancer.

3 Results

This chapter presents the findings on chemical footprint from the literature review, followed by the results of the data collection and resulting CF calculation for USEtox, EF3.1 and ProScale. The ease-of-use of the methods was evaluated, followed by an analysis comparing the CFs from the different LCIA methods. Figure 16-Figure 24 in Appendix C illustrates the results of the CFs for all the methods, for all emission compartments. Finally, results from the LCA are presented.

3.1 Chemical footprint in literature

In five of the articles gathered in the literature review, the concept of chemical footprint was explicitly defined. Zijp et al. (2014) defines chemical footprint as "a *quantitative measure describing the environmental space needed to dilute chemical pollution due to human activities to a level below a specified boundary condition*". Tarasova and Makarova (2016) defines it in a similar way, also including the aspects of space and boundary conditions. Hitchcock et al. (2012), on the other hand, defines it as *"an indication of potential risk posed by a product based on its chemical composition, the human and ecological hazard properties of the ingredients, and the exposure potential during its life cycle."* These definitions are included and referred to in some of the other articles, such as Tarasova et al. (2018) and Brack et al. (2018). The two definitions differ quite a lot. Hitchcock et al. includes the concept of risk and life cycle thinking, not considering space or assimilation capacities like Zijp et al. (2014). Brack et al. (2018) stresses that definitions can differ depending on the situation, for example if the chemical footprint will be assessed for a product or a city, meaning that there can be different definitions depending on the system's scope.

The definitions vary because chemical footprints can consist of different components. Three components that are usually included in the structure of a chemical footprint are risk assessment, life cycle thinking and sustainability assessment in various combinations. Bjørn et al. (2014), Tarasova and Makarova (2016) and Sala and Goralczyk (2013) include all these components, describing the combination of RA with life cycle thinking as the core of the chemical footprint, but also how it can be used to compare (eco)toxicological impacts with environmental boundaries as a kind of sustainability assessment. Tarasova and Makarova (2016) discuss the sustainability assessment by using the planetary boundaries suggested by Rockström et al. (2009) which defines environmental thresholds which outline a safe operating space for humanity with respect to the Earth system and its important functions and processes. Initially, the introduction of planetary boundaries by Rockström et al. (2009) included a planetary system for chemical pollution which lacked a defined limit. This system was later changed into "novel entities", which included the release of *"new substances, new forms of existing substances, and modified lifeforms that have the potential for unwanted geo-physical and/or biological effects"*, but with the boundary still not yet quantified (Steffen et al., 2015). The lack of set threshold values for chemical pollution creates a gap between the use of planetary boundaries and the chemical footprint assessment methods which aim to define a distance to a carrying capacity limit but seem to be used as a sustainability assessment tool in chemical footprint literature anyway. The use of planetary boundaries is also mentioned by Sala and Goralczyk (2013), as an example of how the current or a future

situation should be related to limits of the planet, and thereby assessing the potential harm of the chemical emission.

A regional level sustainability assessment can be included in the chemical footprint by considering environmental conditions in a specific region. Both Sörme et al. (2016) and Erhart and Erhart (2022) addresses a national spatial boundary, using Sweden as an example. Sörme et al. calculates Sweden's chemical footprint in USEtox 1.01. Leclerc et al. (2019) and Tarasova and Makarova (2016) also consider national boundaries, although including all the European countries. Tarasova's and Makarova's assessment is based on the different countries' assimilation capacities, by assessing the ratio between the amount of freshwater in a country and the total chemical pollution.

Some articles describe the chemical footprint as based on two of the three described components. For those, the most common structure presented combines RA and life cycle thinking. This is the case for Hitchcock et al. (2012), Leclerc et al. (2019), Sörme et al. (2016) and Rydberg et al. (2014). Sörme et al. (2016) sees no need to relate a chemical footprint to an environmental threshold, describing it as a stand-alone indicator considering potential impacts from hazardous chemicals emitted during the life cycle of an objects under study.

Combinations of either RA or LCA with sustainability assessment are also mentioned (Brack et al., 2019; Brack et al., 2018; Vanham et al., 2019; Zijp et al., 2014). Focus is then put on relating (eco)toxicity impacts to environmental limits. For instance, Zijp et al. (2014) mentions how chemical pollution should be related to a natural boundary based on the sensitivity of the ecosystem.

Some of the articles make a distinction between the use of pressure and impact in the definition of chemical footprint in connection to LCA. Pressure relates to the stress a human activity puts on a system and is quantified using a limit (e.g. planetary boundary or regional threshold) (Vanham et al., 2019). Impact describes the consequences of said pressure, for example the loss of species as a consequence of chemical pollution, but since it does not consider any thresholds, nothing is said about the severity of the issue. Nordborg and Vanham et al. (2019) refers to pressure as the correct way of defining the chemical footprint, instead of the use of impact that is more connected to an LCA. On the other hand, uses the concept of impact to express the result of the chemical footprint. How well established this distinction between pressure and impact is within the field is unknown.

3.2 Categorization of the LCIA methods

Figure 2 illustrates how the methods were categorized. Seven out of the eight studied methods were placed in the multimedia fate-exposure category. This category implies that the methods are modelled based on indirect exposure, meaning that the substance travels via the environment before reaching its recipient, that can be either a human or an ecosystem. In this category USEtox 2.13 can be found, along with Impact world+, EF3.1 and ReCiPe 2016 v1.1, which are all based on USEtox. EPS, Eco-cost, and Environmental prices can be found in the sub-category referred to as the monetary methods. Eco-cost adds a monetary cost to CFs assessed with EF3.1, which also makes it

a USEtox based method and the same structure for Environmental prices that are based on ReCiPe, making it a USEtox based method. EPS is not USEtox based, but is instead based on "real" impacts, that have been proven and measured. ProScale differs from the other methods, categorizing as a scoring method based on hazard banding. The method is based on direct exposure and uses H-phrases.

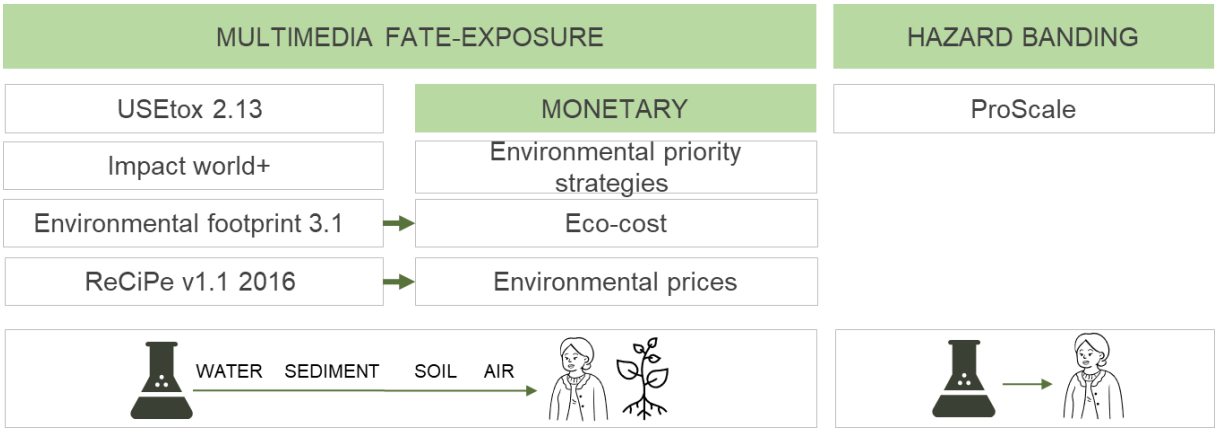

Figure 2. Overview of the categorization made for the methods under study with their associated recipient/-s and exposure pathways. Connections between methods are also indicated with arrows. The USEtox method is also included as the basis for the other methods below it in the column: Impact world +, EF3.1 and ReCiPe 2016 v1.1.

The methods which address ecosystems can also consider different compartments. USEtox 2.13, Impact world + and EF3.1 consider only freshwater aquatic ecosystems (Bulle et al., 2019; Rosenbaum et al., 2008; Saouter et al., 2018), while ReCiPe 2016 v1.1 also considers marine- and terrestrial ecotoxicity (Huijbregts et al., 2017).

3.3 Substance coverage of the LCIA methods

The different LCIA methods tested also cover different groups of substances, which affected the number of CFs from the substance list that could be collected. CFs for all the methods can be found in Appendix C, Figure 16 Figure 24 (for all the compartments, at midpoint level). Figure 3 and Figure 4 illustrates the percentage of collected, calculated, and not found/not possible to calculate CFs for the 73 substances included in the substance list, represented by green, blue and red. Figure 3 shows the substance coverage for ecotoxicity and Figure 4 for human toxicity (including cancer and non-cancer CFs). This grouping is further split into organic and inorganic substances.

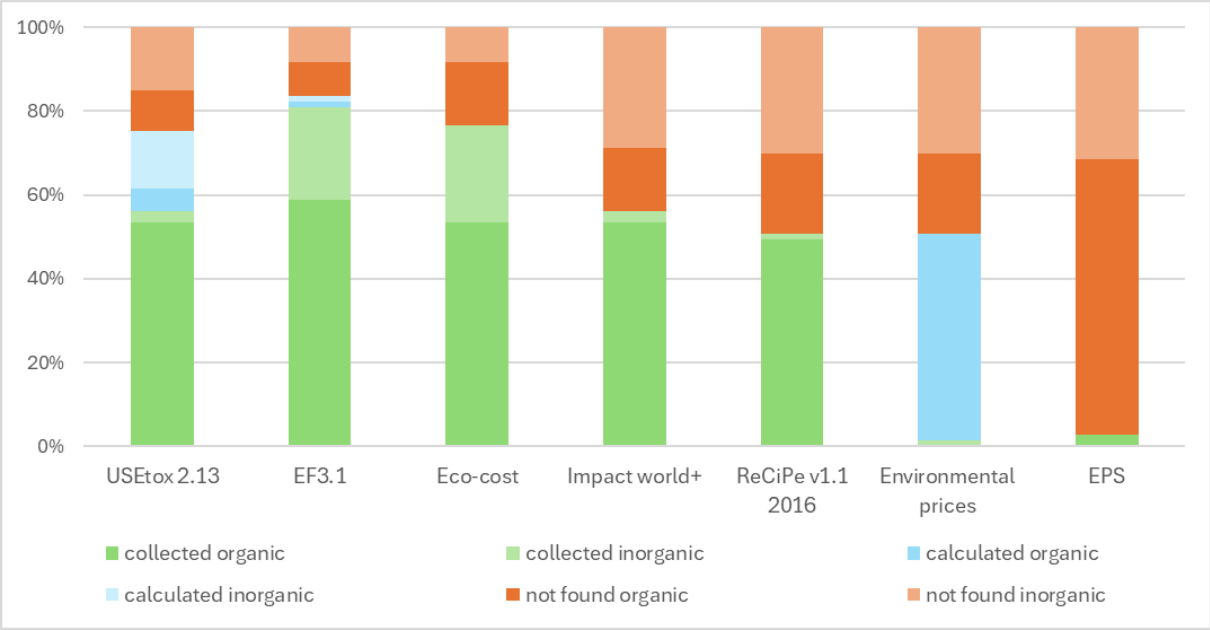

Figure 3. Overview of the substance group coverage of ecotoxicity CFs in the different LCIA methods. Inorganic substances include metals, salts, and elements.

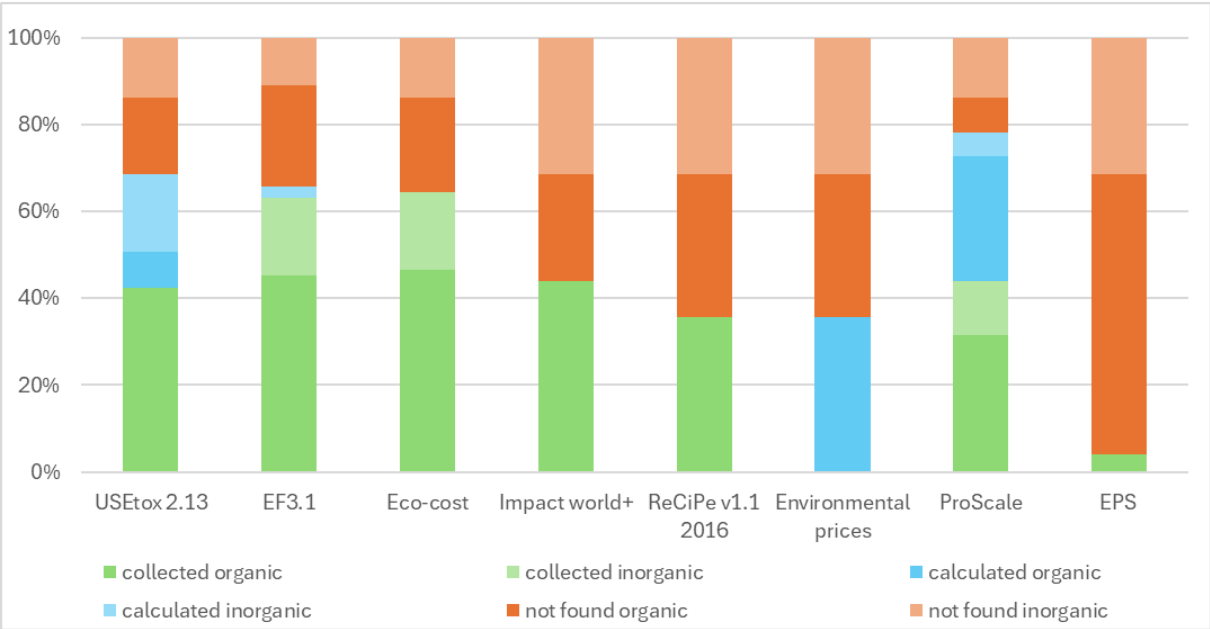

Figure 4. Overview of the substance group coverage of human toxicity – including cancer and non-cancer CFs in the different LCIA methods. Inorganic substances include metals, salts, and elements. A higher percentage of CFs were not found for USEtox and EF3.1 because of a miss in the initial stage of the project, when it was assumed that CFs would be available for both the human toxicity category and the ecotoxicity category if available in the ecotoxicity category, which was checked for predefined CFs. Because of this, it was missed out to calculate some of the CFs since they were assumed to exist.

As can be seen in the figures, the substance coverage of the collected CFs is approximately the same for the multimedia fate-exposure methods USEtox 2.13, EF3.1, Impact world + and ReCiPe 2016 v1.1. EF3.1 has slightly higher coverage since it also covers inorganic substances. For all these methods there is a larger substance cover for ecotoxicity CFs in comparison with human toxicity CFs.

The Eco-cost method cover the same amount of substances as were collected from EF3.1, which is explained by it being based of off the EF3.1 method but with a monetary value added to the substances. The same can be said for Environmental prices and ReCiPe 2016 v1.1, where Environmental prices used the CFs from ReCiPe with a monetary value added. The Environmental prices CFs were all considered as calculated since the ReCiPe 2016 v1.1 CFs were used as a basis for manual multiplication with a monetary value for toxicity impacts. This was done to only include the cost of toxicity impacts and not other environmental issues.

ProScale is only represented in the human toxicity category (since it is the only impact category it covered at the start of this study), showing the highest number of obtained CFs out of all the methods, most for organic substances. The collected CFs in ProScale refers to substances that had prelisted H-phrases in the Excel tool, meaning that these were added automatically by the tool. The calculated CFs refers to a manual collection of the H-phrases. Worth mentioning is that ProScale did not have a list with readily available CFs and for all CFs a minor calculation step was carried out. For inorganic substances, ProScale covers a large number of substances. It covers the same number of substances as USEtox 2.13 when both collected and calculated CFs are included. However, ProScale does not cover as many inorganic substances as the EF3.1 method, which is related to missing H-phrases. The H-phrases can be missing either because the substance has not yet been classified, or because it does not have toxic properties that would result in a hazard classification. EF3.1 covers the highest percentage of substances from the substance list in the ecotoxicity category when both collected and calculated CFs are included. The high coverage is achieved since EF3.1 handles inorganic substances and gives the possibility of calculating new CFs.

The EPS method has the lowest number of found CFs out of the methods in both categories, only two including CFs for ecotoxicity and 3 CFs for human toxicity.

For the substances hydrogen (1333-74-0), nitrogen (7727-37-9), oxygen (7782-44-7), soybean meal (68308-36-1), sulphate (14808-79-8), ESBO (8013-07-8) and calcium chloride (10035-04-8) no CFs were collected or calculated considering all methods.

3.4 Ease-of-use evaluation and overview on how the LCIA methods are described

Table 4 presents a summary of the aspects included in the evaluation of the accessibility and ease-of-use, five aspects have been considered. The first aspect considers if there were predefined CFs that were listed and were possible to collect without calculations or by breaking down the method to extract a CFs (in the case of EPS). Secondly, if a step-by-step guidance on calculating new CFs was available, for example by following a manual or a descriptive report. Third, if the method had a tool for calculating the CFs, for example an Excel tool. The fourth aspect considered the number of parameters required to calculate a CF, including both physio-chemical parameters and scenario-based parameters, for example mass flow. Finally, if the method could be implemented in an LCA that is based on ISO14040 and the potential impact can be expressed at an endpoint level, making it comparable to other environmental issues. These aspects are further commented on in the following sections for each method. For each method a short

background description is also included, followed by the result from the data collection that enabled calculation of new CFs.
Table 4. Usability evaluation aspects for the assessed methods. The evaluation considers five aspects regarding the possibility and procedure for calculating and collecting new CFs, further the number of parameters required in the calculation and also the possibility of using the method in an LCA (following ISO14040).

LCIA method	Database of CF available	Step-by-step guidance	Calculation tool	Parameters needed	LCA implementation
USEtox 2.13	Yes	Yes	Yes	11	Yes
ProScale	No	Yes	Yes	5	No
Environmental Footprint 3.0/3.1	Yes	Yes	No	11	Yes
Environmental Priority Strategies, EPS	No	No	No	-	Yes
Eco-cost	Yes	No	No	-	Yes
Environmental prices	No	No	No*	-	Yes
Impact world +	Yes	No	No	-	Yes
ReCiPe 2016 v1.1	Yes	No	No	-	Yes

**Tool existing for collection of CFs considering the valuation of impacts from all impact categories, but not for only the toxicity impact.*

3.4.1 Evaluation of USEtox 2.13

USEtox is a multimedia fate-exposure model which only considers toxicity impacts (Rosenbaum et al., 2008). It is possible to calculate new CFs using an Excel-based tool. The USEtox 2 method, which only considers indirect exposure, is described in several documents which can be openly accessed. Three manuals are available: one general version (Fantke et al., 2015c), one for organic substances (Fantke et al., 2015d) and one for inorganic substances (Fantke et al., 2015b). Additionally, a more thorough documentation of the model is also provided (Fantke et al., 2017), as well as a manual for the user interface (Fantke et al., 2015a). There is also a newer version of USEtox available, USEtox 3 beta, which also considers direct exposure (Fantke et al., 2021). However, this newer version has not been tested in this thesis project.

In USEtox 2.13, the product of fate, exposure, and effect results in CFs for the impact categories ecotoxicity and human toxicity, which is the sum of the CFs for cancer and non-cancer. Ecotoxicity impacts are expressed as potentially affected fraction of species (PAF) at midpoint and potentially disappeared fraction of species (PDF) at endpoint level. Human toxicity impacts are measured in disease cases at midpoint level and disability-adjusted life-years (DALY) at endpoint level. The CFs also differ depending on the compartment of the emission, including air, surface water and soil (all further differentiated for type and geographic scale).

The method is constructed for organic and inorganic substances, although for inorganic substances only cationic metals are included.

3.4.1.1 Model structure

Out of the 73 substances in the substance list, 32 substances did not have a CF in the USEtox database and had to be calculated. Out of the missing 32 substances, 21 were inorganic and 11 were organic.

The model uses physiochemical properties, fate parameters and toxicity data to calculate a CF. For calculation of new CFs, the required fate parameters are molar mass, chemical class, pKa base reaction, pKa acid reaction, KOW, vapor pressure, solubility, and degradation factors in air, water, sediment, and soil (where degradation rates in sediment and soil can be derived from the degradation rate in water). Bioaccumulation in fish is required for exposure calculation (Fantke et al., 2015c). The effect parameters are based on toxicity data, HC50 (avlogEC50) for ecotoxicity and ED50, inhalative or ingestion, for human toxicity. Additional parameters can be quantified, e.g. partitioning descriptors, but if not available those are calculated by model internal algorithms. All mandatory parameters are described in Table 10 in Appendix A

Figure 5 illustrates the data coverage of the mandatory parameters for the organic substances that were missing in USEtox 2.13. However, since inorganic substances have been assessed using the methodology for organic substances, the parameter coverage include those substances as well. The data are described as experimental, predicted, or not found. The experimental data refer to found data that were labeled experimental. The predicted data includes both found data that were labeled predicted and data that were generated (predicted) in the tool EPI Suite (United States Environmental Protection Agency, 2012). The data coverage of the mandatory parameters is further divided into showing the coverage for organic or inorganic, respectively.

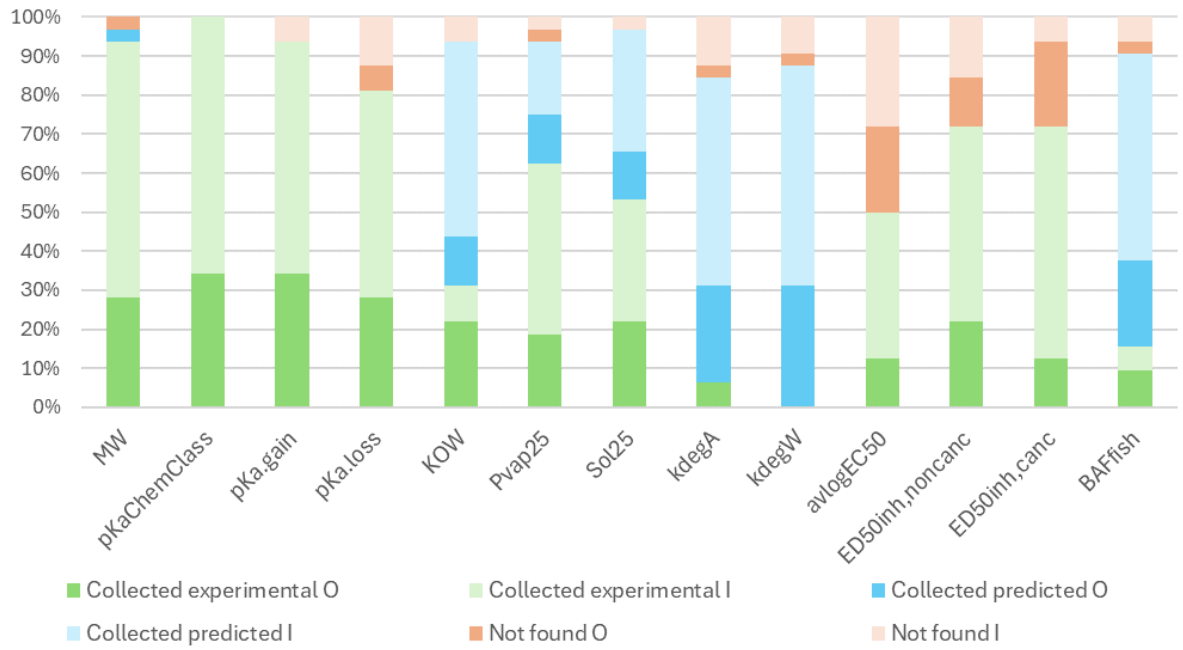

Figure 5. Overview of the data coverage and data type for the required parameters in USEtox 2.13. The data collection was made for the 32 substances from the substance list that were missing CFs in USEtox 2.13. O = organic substances; I = inorganic substances.

The fate parameters molar weight and pKa show a high percentage of found data. For the parameter K_{OW} the graph shows a small amount of experimental inorganic data points, so a large amount of the inorganic K_{OW} data points had to be predicted or were already labeled as predicted upon collection. For the parameter solubility, approximately half of the data points were experimental, and half predicted. The coverage is similar for the K_{OW} parameter, but with slightly more experimental values found. For the degradation parameters (k_{degA} and k_{degW}) a high share of data were predicted. Additionally, not all sources explicitly stated if the data were experimental or predicted, which could introduce further uncertainties. The figure further shows that less toxicity data was found for ecotoxicity ($avlog_{EC50}$) in comparison with human toxicity parameters ($ED_{50,\ cancer}$ and $ED_{50,\ non\text{-}cancer}$). Out of the found $ED_{50,\ cancer}$ data points, all were zero except for one substance, zero meaning that these substances are expected not to be carcinogenic and the "not found" represents a data gap.

3.4.1.2 Accessibility and ease-of-use

The main document used herein was the general manual (Fantke et al., 2015c). The manual was structured in an easy-to-follow manner, covering all parameters/calculations needed for the calculation of new CFs. However, it was not always clear what parameters were required or the hierarchy of different data points when consulting different documents. For instance, pKa chemical class, base reaction and acid reaction are said to be mandatory parameters for organic substances in the manual but said not to be required in the longer documentation, where it is described that these parameters will be set to specific values if left blank. Additionally, the instructions on if bioaccumulation factors (BAF) are required or not are not clear. The manual states that the BAF parameters are not required, but also mentions that they are needed for calculation of human exposure factors (Fantke et al., 2015c). It is also said that BAF for organic substances can be estimated based on K_{OW}.

The manual describes a clear hierarchy regarding type of toxicity data, which was easy to follow if data were found for the allowed points of departure types, using the correct units. For human toxicity tests, the manual mentioned ED_{50}, NOAEL, NOAEC, LOAEL and LOAEC as points of departure that could be used for calculation of new CFs. The USEtox 2.13 tool on the other hand, could also make use of LD_{50}, EC_{50} and TD_{50} values, none of which were mentioned as acceptable points of departure in the manual but described in the longer documentation (Fantke et al., 2017).

Inhalation data were often given as NOAEC or LOAEC values, which are points of departure mentioned in the manual, but not possible to add directly into the excel template without prior conversions. Only EC_{50} values were considered to have an inhalation rate in the template, meaning NOAEC or LOAEC values had to be converted into EC_{50} values before insertion into the USEtox 2.13 Excel tool. Since these conversions were not described in the manual, a strategy to handle a lack of information was derived (a structure was established for this thesis). The assumptions and calculations are described in section 2.4.1.

The evaluation of which toxicity data to use, i.e., which toxicity tests generate relevant data for this purpose, was challenging without in depth knowledge in toxicology. The biggest struggle was choosing tests with relevant adverse endpoint effects, filtering out those effects that might have been measured, but does not result in an adverse outcome for the organism/ecosystem relevant in this context. It was also challenging to decide on which the most sensitive effect was. The identification of the most sensitive effect was needed according to the manual to derive human health relevant ED50 values. On the ecotoxicity side the most sensitive effect was used to ensure that relevant data were used where several effect endpoints were reported from the same test (e.g. by excluding less sensitive weight gain effects from a reproduction toxicity study).

3.4.2 Evaluation of Environmental footprint 3.1

EF3.1 is part of the product environmental footprint (PEF) method, which considers 16 impact categories relevant in an LCA. PEF is developed by Joint research center (JRC) and is the LCA method advised by the European commission to use when conducting an LCA in the EU (Zampori, 2019). The method compiles already existing LCIA methods and recommends which one to use for each impact category, although in the case for (eco)toxicity alterations to the method are made. The LCIA method for (eco)toxicity is based on USEtox 2.1 with alterations considering the data collection and the ecotoxicity effect data (Saouter et al., 2018). During the pilot phase of the PEF method, difficulties regarding the interpretation of the USEtox method and its result emerged, which resulted in these mentioned alterations.

The CFs have the same units as in USEtox, although the emission compartments differ slightly. Another difference is the substance coverage, as EF3.1 includes inorganic substances by application of a robustness factor to allow for substances outside the applicability domain of the model.

3.4.2.1 Model structure

Out of the 73 substances on the substance list, 14 substances were missing CFs in EF3.1. Out of these 14 substances, 6 were inorganic and 8 were organic. As the EF method is based on USEtox, the same parameters are used. The difference lies within the data collection method and ecotoxicity data value used.

Figure 6. Overview of the data collection source for the required parameters in EF3.1, where REACH is the data source requested in the method. The data collection was made for the 14 substances from the substance list that were missing CFs in EF3.1. O = organic substances; I = inorganic substances. illustrates the parameter coverage based on different data collection sources for these 14 substances. The data collection strategy for EF3.1 is described in section 2.3. The green color illustrates data collected from the highest prioritized database for EF3.1, REACH/ECHA (European Chemicals Agency, n.d.). Data collected from that source will hereon be referred to as REACH data. The blue represents the data collected with other sources, according to the database priority list for EF3.1. These lower ranked databases are outside of the intended use for EF3.1. Data collected from EPI suite is included in the "other sources" despite that using EPI suite as a data source is part of the EF3.1 method.

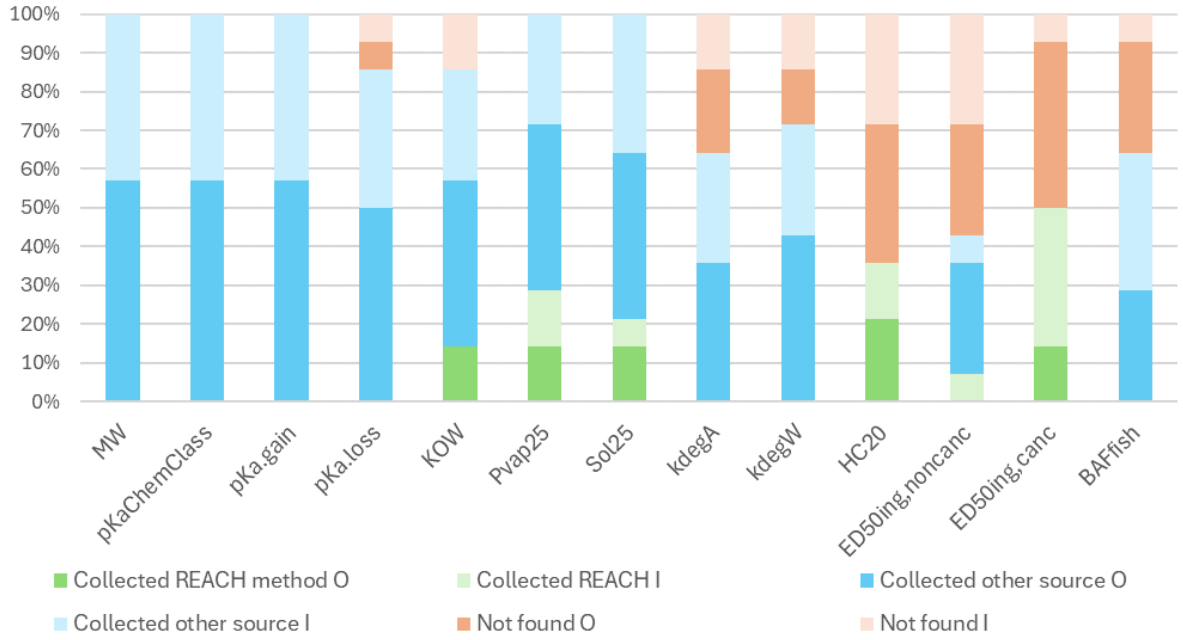

Figure 6. Overview of the data collection source for the required parameters in EF3.1, where REACH is the data source requested in the method. The data collection was made for the 14 substances from the substance list that were missing CFs in EF3.1. O = organic substances; I = inorganic substances.

The figure shows that REACH data were only possible to collect for six out of the 13 required parameters. For all the parameters for which REACH data were available, the coverage is still low, meaning that the database did not have the required data readily accessible. Instead, other data sources had to be used, but this meant departing from the method instructions. However, since only a small number of substances were studied here, the results do not represent the general data availability from REACH.

3.4.2.2 Accessibility and ease-of-use

The EF3.1 method is based on USEtox, there is no manual although a thoroughly informative report (Saouter et al., 2018). The article describes which alteration that has been made in USEtox 2.1 (Fantke et al., 2015c; Rosenbaum et al., 2008) instead of a description of how to handle a new method in full. The article is structured and clear, sometimes describing the USEtox 2.1 in a more comprehensive way than the actual USEtox manual. Furthermore, data choices and alterations made are well described. For example, it is described how to deal with test results that are reported as ranges, how to manage data gaps and how to choose toxicological data. There is no specific tool for the method. Although new CFs can be calculated by following the instruction in the article and then using the USEtox Excel tool (Rosenbaum et al., 2008). Following the instructions from the EF report it should be possible to replicate the EF CFs. This was however not done for this thesis project. The calculations of CFs in EF3.1 are based on an older version of USEtox (USEtox 2.1) than what was used for this project. Since only information on data choices and calculations are described in the report by Saouter et al. (2018), and not the adjusted tool that they used, exact replication can be challenging.

The method is USEtox based, resulting in the same required parameters, although with some alterations and there are also some parameters alterations that has not yet been implemented, although are considered as "work in progress", for example removing the bioaccumulation factor (Saouter et al., 2018). For the ecotoxicity effect data that is an already implemented alteration, one of the challenges found in the EF3.1 manual was how to construct a species sensitivity distribution curve, which was needed to achieve an HC_{20} value for ecotoxicity. The construction of such a curve was not described in the manual. Instead, considering the scope of this thesis, extrapolations were made from already attained HC_{50} values from when calculating CFs in USEtox 2.13 (Rosenbaum et al., 2008). Extrapolation factors for this extraction for different substance groups were given in the manual, this was however the least preferred option for how to achieve HC_{20}. To follow the EF3.1 method fully, a change of value should also have been made in the USEtox 2.13 Excel tool (Rosenbaum et al., 2008) for this ecotoxicity effect factor calculation step. Where USEtox 2.13 calculated the ecotoxicity effect factor by dividing 0.5 with a HC_{50} value, it should instead be reached by dividing 0.2 with HC_{20} in EF3.1 (European Commission et al., 2023). Since the tool used for the derivation of EF3.1 CFs is not available, instead manual changes have to be made to the USEtox Excel tool (Rosenbaum et al., 2008) using adjustment instructions from different sources, it is challenging to follow the method as it is intended to be used.

The CFs were easily extracted from already calculated CFs. Instructions on how to interpret the CFs, regarding emission compartments in comparison with the USEtox emission compartments was easy to understand in the article (Saouter et al., 2018).

3.4.3 Evaluation of ProScale

The ProScale method has a different structure than USEtox and does not generate straightforward CF in the same way, but instead results in a ProScale score. However, in this report, the ProScale score will be referred to as a CF for simplicity reasons. In comparison with USEtox, ProScale is structured to include direct exposure from an industrial, consumer or professional perspective. The required parameters are based on a modelled scenario, considering parameters such as MF, PHF and PROC, combined with

vapor pressure or dustiness of the substance (depending on if the substance studied is a fluid or solid) and H-phrases. The MF, PHF and PROC were all selected to have the same value or process type for all substances in the substance list, to achieve the same exposure scenario and best reproduce a CF. The selected values and PROC are described in section 2.4.3.

The hazard assessment of the method is based on the Globally Harmonized System for the Classification and Labelling of Chemicals (GHS) (Winder et al., 2005). It is a system established by the United Nations, resulting in H-phrases. Instead of collecting toxicity data, an assessment is executed systematically by experts and the substance is labelled with one or more H-phrases. The H-phrases used in ProScale are both harmonized/classified substances or REACH registrants' dossiers notifications, meaning that these substances have been evaluated as hazardous and assigned an H-phrase, although these substances have not been harmonized/classified.

The values chosen for the scenario-based parameters were chosen to come as close as possible to a CF which could be compared with the other methods that were tested. The score has no unit, although similar to the CFs, a higher score indicates a larger toxicity potential.

3.4.3.1 Model structure

Out of the 73 substances on the substance list, hazard statements had to be added manually into the Excel tool for 31 substances. For the rest of the substances, H-phrases were filled in automatically based on the CAS-number. Out of the 31 substances, 11 were inorganic and 20 were organic. The dustiness parameter only applied to the solid substances, these being 29 substances, whereof 18 organics and 11 inorganics.

Figure 7 illustrates the data coverage of the required substance specific parameters for the calculation of ProScale score, described as collected experimental, collected predicted or not found for the parameters vapor pressure and dustiness. The data collection for H-phrases are divided between collected automatically, collected manually or not found. This grouping is further split into organic or inorganic. For the parameter of dustiness all data were considered to be predicted.

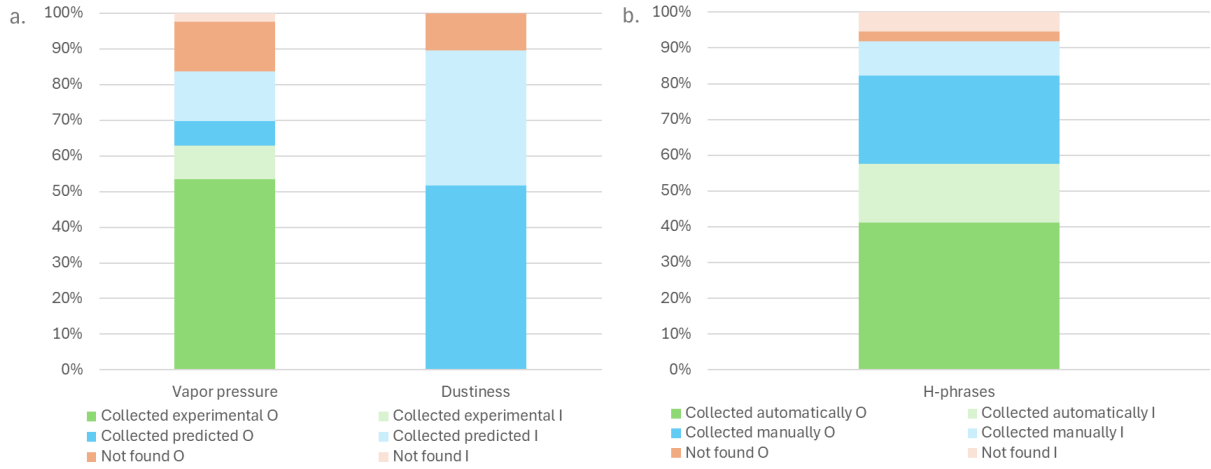

Figure 7. Overview of the data coverage for the required parameters in ProScale. The data collection was made for the 31 substances from the substance list that were missing H-phrases in the ProScale Excel-based tool. O = organic substances; I = inorganic substances.

Vapor pressure was required for all the substances and since it is a common parameter, data were available for most of them. Likewise, the H-phrases had a high coverage when counting both the H-phrases that were already defined in the ProScale Excel tool version 1.6 and the H-phrases that were added manually into the Excel tool. The high coverage of H-phrases is likely due to most of the substances on the substance list being out on the market, and therefore classified. The substances for which H-phrases were not found could either be not classified yet, or harmless enough to not get a hazard classification, but the division between these two scenarios has not been further investigated. The dustiness parameter has a high substance coverage percentage, although it should be considered with high uncertainty, as the dustiness for the substances are not based on experimental tests but rather on their similarities with the examples listed in the method section 2.3.1.1.

3.4.3.2 Accessibility and ease-of-use

The ProScale method is explained by the ProScale guidance document, that was categorized as a manual (Lexén et al., 2021). The model structure is explained in a comprehensible way, making it easy to follow. For this thesis, ProScale did not offer calculated CFs, instead the score was calculated in an Excel tool. It was easy to use the tool and to understand the result. As the method only assesses the impact category of human toxicity, the manual is based on this which makes the instructions easy to follow.

The ProScale model only required entry or selection of five parameters to calculate a score corresponding to a characterization factor. Most of the parameters are well explained and easy to assess. However, the description of the dustiness parameter for solid substances, was not adequate to assess dustiness of a substance without difficulties. The different levels of dustiness are only briefly defined by other typical materials that fall under that category. Without a property that can be given as a number to refer to, it was difficult to decide on which level each solid substance belonged to.

Toxicity data is included in ProScale by the use of H-phrases. There, the toxicity data are already assessed by a professional doing the classification, which avoids the need for the LCIA operator to make the evaluation of the data. This made the use of the data and the calculations easier than in e.g. USEtox 2.13, where toxicity data had to be valuated and adjusted manually.

3.4.4 Evaluation of Environmental priority strategies

The EPS is an LCA method, resulting in an environmental load based on "actual" impacts from different impact categories, aiming at covering all environmental impacts observed globally. "Actual" impacts refer to measured data from scientific studies for a specific substance. For example, the assessment of years of lost life (YOLL, equal to DALY) per kg Benzene includes an estimation of the number of cancer cases based on the Benzene concentration in air. Further, an estimated exposure is found, based on a study of six European cities. Finally, the assessment includes a number on the amount of Benzene emitted yearly globally.

Instead of the commonly used impact categories of ecotoxicity and human health (cancer and non-cancer) the substances are divided into emission groups, such as volatile organic compounds (VOC) or pesticides. The calculations differ between the emission groups, although all consider aspects such as fate, exposure and effect but in different constellations.

The CFs for (eco)toxicity obtained from the method was expressed in DALY for human toxicity and normalized extinction of species (NEX) for ecotoxicity, this is an indicator based on Swedish measurements of the "willingness to pay" for avoiding the extinction of species per year on a global basis (Steen, 1999). By extracting the CFs for (eco)toxicity the monetary evaluation was excluded, although could be added by following the instructions for the cost of 1 DALY and 1 NEX. The method includes organic and inorganic substances, including metals. The EPS method offers no description on calculating new CFs, but instead recommends the use of proxy substances (Steen, 2019), and therefore no data was collected.

3.4.4.1 Accessibility and ease-of-use

Documentation of the model structure was available, describing the data and correlations that were used as a foundation for the monetary evaluations (Steen, 1999, 2019). The method as a whole is thoroughly explained, although for the purpose of this thesis, to find CFs for (eco)toxicity and how to extract these were not included in the method's instructions.

An Excel tool stored all the environmental scores for the substances assessed in the EPS. The Excel tool was not very clear as it was divided based on the different emission groups, resulting in different designs that were perceived as not very approachable. It was hard to grasp where in the model (eco)toxicity was considered as it was not explicitly stated. Once the (eco)toxicity was found it was a challenge to understand how to withdraw CFs that could be used in this thesis, mainly because the calculation differed depending on which emission group the substance belonged to.

Difficulties arose in understanding the parameters included in the cause-effect chains as it is very case dependent. The same endpoints/indicators had different pathways or the other way around. Therefore, it was challenging to understand what category to use as the CF and how to interpret it.

No calculations were made, as the method does not enable the calculation of a environmental load unit (ELU) for new substances. In the complementary literature it is mentioned that new ELUs should not be made, and it is recommended as instead making a proxy, arguing that all important substances are considered. The procedure for adding substances would be too comprehensive as it needs to be carried out by an expert within the area.

3.4.5 Evaluation of other USEtox-based methods

This section will evaluate the experience of obtaining CFs for (eco)toxicity from the USEtox based methods Impact world +, ReCiPe 2016 v1.1, Eco-cost and Environmental prices (excluding EF3.1 which has already been covered). All these methods are based on USEtox, but with targeted alterations made. Impact world + uses USEtox as its base,

although it emphasizes the spatial differences in the model, by using continent-specific factors. ReCiPe uses the USEtox database and method as a foundation, although alterations based on the method USES-LCA are integrated in the method, these alterations consider a few different aspects, such as the handling of dissociated substances, for example affecting parameters such as the BCF_{fish}. Eco-cost and Environmental prices are both monetary methods, which are based on two of the USEtox-based methods. Eco cost uses EFs CFs and translates them into a cost, whilst Environmental prices use ReCiPe's CFs. Impact world + is measured in the same units as USEtox, i.e. cases and PAF or DALY and PDF. ReCiPe's midpoint CFs are instead measured in 1,4-dichlorobenzene-equivalents (1,4 DCB-eq) and DALY for the endpoint CFs. Eco-cost and Environmental prices are measured in euros. The emission compartments differ slightly, all methods include emissions to air, water, and soil, although the specific categories within these groups can differ between one another and in comparison with USEtox despite it being the base model.

3.4.5.1 Accessibility and ease-of-use

All methods instructions except Eco-cost were found in articles, Eco-cost instead had a website. Common for all these methods is that the articles/website includes the procedures for all the impact categories part of an LCA, which makes it challenging to find the information on (eco)toxicity specifically.

All the tools except for Environmental prices had Excel tools with CFs listed and ready to be collected for the substances. Environmental prices had CFs that included all impact categories, so to attain only (eco)toxicity CFs, ReCiPe's CFs were multiplied with a monetary factor (de Bruyn et al., 2018).

All the methods are based on USEtox and therefore requires the same parameters. For these methods no new CFs were calculated, as they were not prioritized for the assessment (see 2.2.1) but also because instructions for such calculations were not available for all methods. Some calculations were however made, for Environmental prices, for which a monetary value was added to the already collected CFs from ReCiPe 2016 v1.1. It would be possible to add CFs for Eco-cost for the new CFs calculated with EF3.1, as a factor could be extracted from the Eco-cost website and multiplied with the EF3.1 CFs but this was not done herein. No attempt was made at calculating new CFs for Impact world+, as it was difficult to understand in what way the USEtox model was used, for example if there were certain parameters that were changed or added in Impact world + from reading the manual and it would therefore be challenging to calculate new CFs. Likewise for ReCiPe it was difficult to understand how the parameters were used as the method is a mix between USEtox and USES-LCA and calculating new CFs would be challenging.

3.5 Comparison of characterization factors across LCIA methods

In the following chapter the methods are analyzed by comparing their CFs. The higher the CF, the higher the potential (eco)toxicity impact potential.

3.5.1 Comparison of the USEtox-based methods

This chapter will compare the USEtox-based methods based on their CFs. Figure 8 and Figure 9 illustrates normalized and logarithmic CFs from USEtox 2.13, EF3.1, ReCiPe 2016 v1.1 and Impact world + for ecotoxicity and human toxicity (combined cancer and non-cancer). The substances for which CFs have been calculated as a part of this thesis project in USEtox 2.13 are marked in the figure with an asterisk (*) at their CAS number. Similarly for the substances calculated with the EF3.1 method, although these are marked with (**).

Inorganic substances covered here have been calculated despite of them falling outside the applicability of USEtox 2.13. Additionally, the inorganic substances were calculated for using the same data and strategy as for organic substances instead of the strategy for inorganic substances in USEtox, which only handles cationic metals. This strategy was implemented since the required parameters for inorganic substances were difficult to find, so to be able to calculate CFs for any inorganic substances, they were assessed as organic substances. Because of this strategy, the inorganic substances assessed should be seen as highly indicative and not be given much weight when comparing and analyzing the results. This is the case for all inorganic substances seen in the figures except for sulfuric acid (CAS: 7664-93-9), for which it was indeed found a CF for in the ecotoxicity impact category in the organic USEtox 2.13 database (Rosenbaum et al., 2008).

As can be seen in Figure 8, the midpoint CFs for human toxicity for emissions to air from USEtox 2.13, EF3.1, ReCiPe 2016 v1.1 and Impact world+ all follow a similar pattern for the organic substances. This pattern can also be seen for ecotoxicity in Figure 9. This is also visible for the emission compartments water and soil, that are not presented here, although can be found in Appendix C, Figure 16-Figure 24.

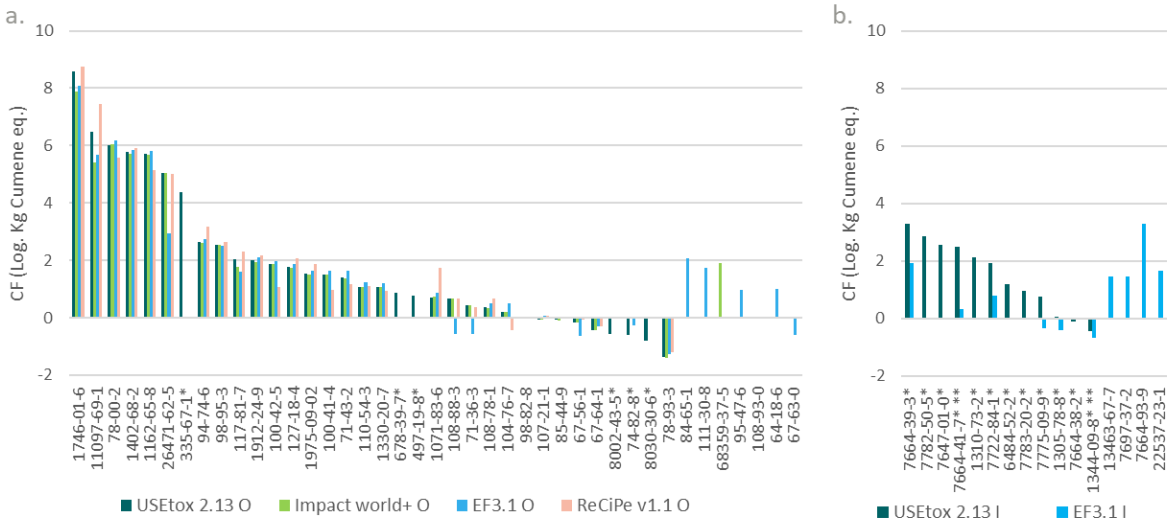

Figure 8. Midpoint, human toxicity (non-cancer and cancer) CFs from USEtox 2.13, Impact world +, EF3.1 and ReCiPe 2016 v1.1 for the emission compartment air, normalized to the substance cumene (CAS: 98-82-8). Sorting based on CFs from/calculated based on USEtox 2.13, high-to-low. Only substances with a CFs are presented in the graphs. CFs calculated

as part of this thesis project based on USEtox 2.13 are indicated with an * in connection to the substance's CAS number. CFs calculated as part of this thesis project based on the EF3.1 method are indicated with ** in connection to the substance's CAS number. Inorganic substances (except cationic metals) outside the applicability domain for USEtox 2.13.

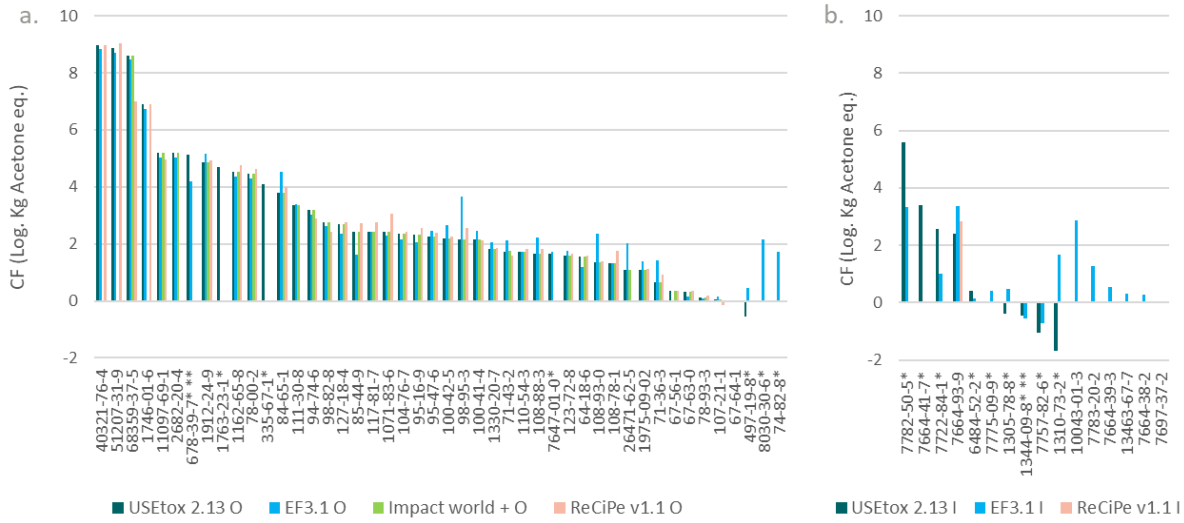

Figure 9. Midpoint, freshwater ecotoxicity CFs from USEtox 2.13, Impact world +, EF3.1 and ReCiPe 2016 v1.1 for the emission compartment air, normalized to the substance acetone (CAS: 67-64-1). Sorting based on CFs from/calculated based on USEtox 2.13, high-to-low. Only substances with a CFs are presented in the graphs. CFs calculated as part of this thesis project based on USEtox 2.13 are indicated with an * in connection to the substance's CAS number. CFs calculated as part of this thesis project based on the EF3.1 method are indicated with ** in connection to the substance's CAS number. Inorganic substances (except cationic metals) outside the applicability domain for USEtox 2.13.

3.5.1.1 Parameters evaluation

To facilitate understanding of what substance property parameters that influence the characterization factors,

Table 5 and Table 6 show the relation of the physiochemical property and toxicity parameters for the seven substances with the highest ranked CFs in the human toxicity and ecotoxicity categories, respectively, compared to the 5th and 95th percentile for the same parameter in the USEtox database. The percentiles are based on the database of the substances listed in USEtox 2.01, which concludes 3082 substances (Hauschild et al., 2017). The blue color indicates that the property value for the substance places in the 95th percentile of the range of values for the given property. The purple color indicates that the property value for the substance instead places in the 5th percentile of the range of values for the property studied. The grey colored boxes indicate that that property is not applicable for the toxicity category in focus. If no color is assigned, the property value falls between the 5th and 95th percentile.

Table 5. Analysis of the physiochemical and toxicity properties of the substances from the substance list with the seven highest CFs with respect to the 5th or 95th percentile in the human toxicity category.

Substance	2,3,7,8-TetraCDD	AROCLOR 1254	Tetraethyl lead	AFLATOXIN	Aflatoxin B1	2,4/2,6-TOLUENE DIISOCYANATE	PFOA
CAS number	1746-01-6	11097-69-1	78-00-2	1402-68-2	1162-65-8	26471-62-5	335-67-1
MW							
K_{OW}	>95	>95					
P_{vap}							
Sol	<5	<5	<5				
k_{degA}				>95	>95		
k_{degW}	<5	<5					
BAF_{fish}	>95	>95					>95
$avlog_{EC50}$							
$ED_{50,\ non\text{-}canc}$		<5	<5	<5	<5	<5	
$ED_{50,\ canc}$	<5			<5	<5	>95	<5

Table 6. Analysis of the physiochemical and toxicity properties of the substances from the substance list with the seven highest CFs with respect to the 5th or 95th percentile in the ecotoxicity category.

Substance	1,2,3,7,8-PENTACHLORODIBENZO-P-DIOXIN	CYFLUTHRIN	2,3,7,8-TetraCDF	3(2H)-ISOTHIAZOLONE,2-METHYL-	8:2 FTOH	2,3,7,8 TetraCDD	AROCLOR 1254
CAS number	40321-76-4	51207-31-9	68359-37-5	2682-20-4	678-39-7	1746-01-6	11097-69-1
MW		>95			>95		
K_{OW}	>95		>95			>95	>95
P_{vap}							
Sol	<5	<5	<5			<5	<5
k_{degA}					<5		
k_{degW}	<5	<5	<5			<5	<5
BAF_{fish}	>95		>95			>95	>95
$avlog_{EC50}$	<5	<5	<5			<5	<5
$ED_{50,\ non\text{-}canc}$							
$ED_{50,\ canc}$							

The two tables show that for some parameters the substances with the highest CFs tend to have a value that is included in either the top or the bottom percentile. These tendencies are the clearest for the human toxicity effect parameters (ED_{50}) for the

human toxicity category (where a low ED_{50} value indicates a high toxicity) and for the ecotoxicity, the ecotoxicity effect parameter, but also degradation in water and water solubility parameters for the ecotoxicity category. The fact that the toxicity parameters are important parameters in both categories show the importance of correct use of (eco)toxicity data.

Degradation in water and water solubility relate to the fate of the substances in the water. A low degradation in water as the substances show means that the substances will not be, or only over a long time, degraded in water. This persistency will cause the substances to accumulate in the environment, which will in turn result in a higher degree of exposure to the substance. They also show a low solubility in water, which in turn mean that they are more likely to dissolve and accumulate in hydrophobic solutions, like fatty tissue. This distribution between water and hydrophobic solutions, like octanol, connects to the K_{OW} parameter, which tend to have a high value for the studied substances. This can lead to the substances accumulating in the fatty tissue, building up the concentration of the substance in an organism to a level that can be of risk, resulting in a high ecotoxicity effect.

The three highest CFs for inorganic substances were also analyzed based on the same method. However, this result is not presented herein due to lack of patterns noted, except for a high effect parameter for (eco)toxicity leading to a high CF, although no values were above the 95-percentile.

3.5.1.2 Differences in results due to structure variations of the models and required input parameters

The three methods cover mainly the same substances, with a few exceptions. This overlap is expected since toxicity impacts in both EF3.1, ReCiPe 2016 v1.1 and Impact world + build on the USEtox model.

Impact world + is based on a parameterized version of USEtox for continents (Bulle et al., 2019) meaning that the USEtox method was assigned new parameters related to continental differences, mainly in connection to freshwater pathways. Comparing the relation between USEtox and Impact world+ for human toxicity there is a tendency for slightly lower values, although many of the values are very similar. By investigating the differences further, by comparing cancer and non-cancer in Appendix C Figure 16 – Figure 24, the Impact world+ cancer values had a tendency to deviate more, resulting in lower values than the non-cancer values, especially for the soil emission compartment. In ecotoxicity there is no deviation.

CFs calculated with EF3.1 also follow the trend of USEtox, with slight deviations both for ecotoxicity and human toxicity, resulting in both lower and higher values in comparison with USEtox. In Appendix C Figure 16 – Figure 24, EF3.1 shows lower values in the cancer impact category. This difference could be because the USEtox version 2.13 has been used in this report whereas USEtox version 2.1 was used to calculate the CFs with EF3.1. For the human toxicity non-cancer the deviation, resulting in lower values, probably depends on the use of REACH data. For ecotoxicity the differences are more scattered, resulting in CFs with much larger values in comparison with USEtox. This is probably due to the

toxicity effect factor HC_{20} instead of HC_{50} that is used in USEtox. Comparing the inorganic substances no tendencies can be observed, as there are too few substances assessed by both USEtox 2.13 and EF3.1. In EF3.1 a robustness factor was added to cope with the lack of inclusion of different behavior of degradation or dissociation by inorganic substances. If more inorganic substances could have been assessed maybe there could have been a tendency that the EF3.1 CFs would have been lower regarding the robustness factor.

ReCiPe 2016 v1.1 deviates in the human toxicity impact categories in the sense of higher CFs, what this is based on has not been able to identify. Although comparing the different emission compartments in Appendix C Figure 16 - Figure 24, ReCiPe v1.1 had higher CFs in the air compartment (human cancer and human non cancer) compared with USEtox, the soil compartment in the same impact categories had higher values for human non cancer and lower for human cancer. For the water compartment the values were more similar. Analysing the ecotoxicity, ReCiPe v1.1 had higher values than USEtox in the air compartment, lower in the soil compartment and similar in the water compartment.

3.5.2 Comparison of methods based on different model structures

Two methods that differ a lot in input data and model structure and scope are USEtox 2.13 and ProScale. USEtox 2 is a multimedia fate model which considers indirect exposure, while the ProScale model predicts impacts on human health followed by direct exposure. These differences result in visible differences to the obtained CFs for the different substances assessed in the study. The variations in the CFs obtained in USEtox 2.13 and in ProScale are depicted in Figure 10.

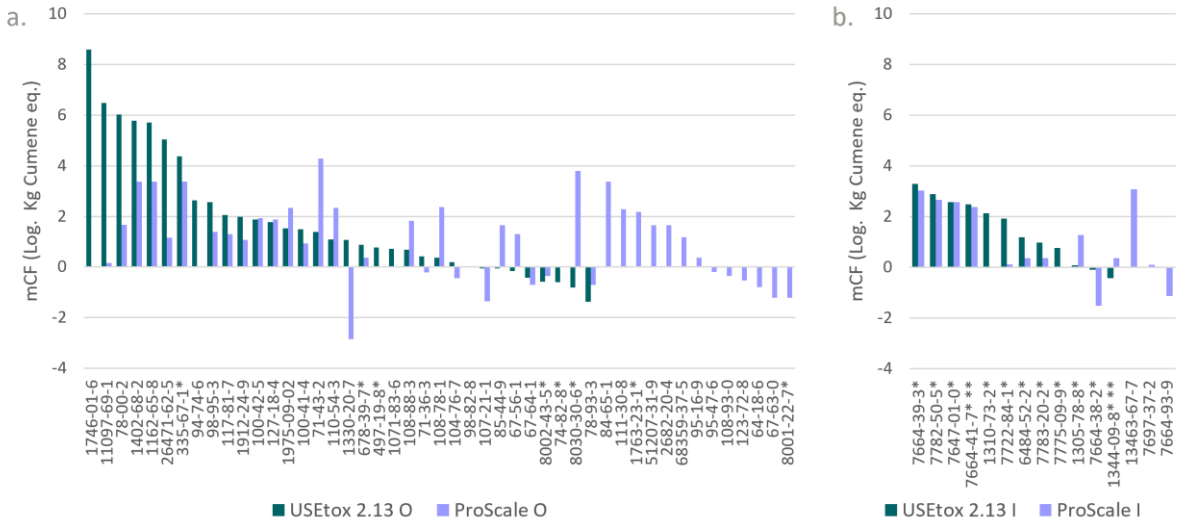

Figure 10. Midpoint, human toxicity – non-cancer CFs from USEtox 2.13, and ProScale for the emission compartment air, normalized to the substance cumene (CAS: 98-82-8). Sorting based on CFs from/calculated based on USEtox 2.13, high-to-low. Only substances with a CFs are presented in the graphs. CFs calculated as part of this thesis project based on USEtox 2.13 are indicated with an * in connection to the substance's CAS number.

As shown in the figure, the CFs in USEtox 2.13 and ProScale do not follow a common pattern for most of the substances. However, a similar tendency can be detected for the four most hazardous inorganic substances, which both USEtox 2.13 and ProScale rank in the same order. This is notable, since the inorganic substances in USEtox 2.13 have been calculated outside of the model domain as a test, and therefore possess an inherent

uncertainty. Also, the organic substances styrene (CAS: 100-42-5) and tetrachloroethylene (CAS: 127-18-4) are assessed to have a similar impact in both USEtox 2.13 and ProScale. Outside of these substances, no similarities can be detected, with the CFs varying in size. Within the methods themselves, USEtox 2.13 portray bigger variations in the size of the CFs, taking on bigger extremes, while the CFs from ProScale take on less extreme values.

The ProScale scores for the organic substances however do not follow the same hazard ranking as the three substances with the highest CFs in USEtox 2.13. As can be seen in the figure, the most hazardous substance in the category according to USEtox 2.13 is not assigned a score in ProScale. This is because its classifications only connect to oral and dermal exposure, not inhalative which is the exposure pathway used for the comparison of USEtox 2.13 and ProScale. The second most hazardous substance in USEtox 2.13 is only given a minor score in ProScale, indicating that it would not be very toxic if emitted. The opposite can be seen for the second most hazardous substance in ProScale, naphtha (CAS: 8030-30-6) is given a minor score in USEtox 2.13. This might be due to the differences in exposure that the two methods consider. Naphtha is approximated to biodegrade in water in six hours, according to EPI suite (United States Environmental Protection Agency, 2012), which results in a low indirect exposure level in USEtox 2.13. On the other hand, when considering direct exposure to naphtha in ProScale, it can be ranked as more harmful since it is classified as an aspiration hazard with carcinogenic and mutagenic properties (European Chemicals Agency, n.d.), which is why the substance is given a higher score and higher ranking.

The figure shows big differences between USEtox 2.13 and ProScale. Like for the example with naphtha, this might be because USEtox 2.13 handles indirect exposure to humans via the environment, while ProScale considers direct exposure to industrial workers (used for the CFs above), professional workers or consumers and hence the two methods intend to answer different questions. The deviating results could also be due to difference in input data where ProScale also depends on the chosen MFs, PHFs and PROCs and USEtox make use of a different data input.

3.5.3 Comparison of methods at an endpoint level

Endpoint CFs were obtained for four (USEtox 2.13, Impact world +, EPS and ReCiPe 2016 v1.1) out of the eight assessed LCIA methods. For the remaining three methods (ProScale, EF3.1 and Eco-cost) endpoint CFs did not exist. The endpoint CFs are given in disability-adjusted life years (DALY) and are shown in Figure 11.

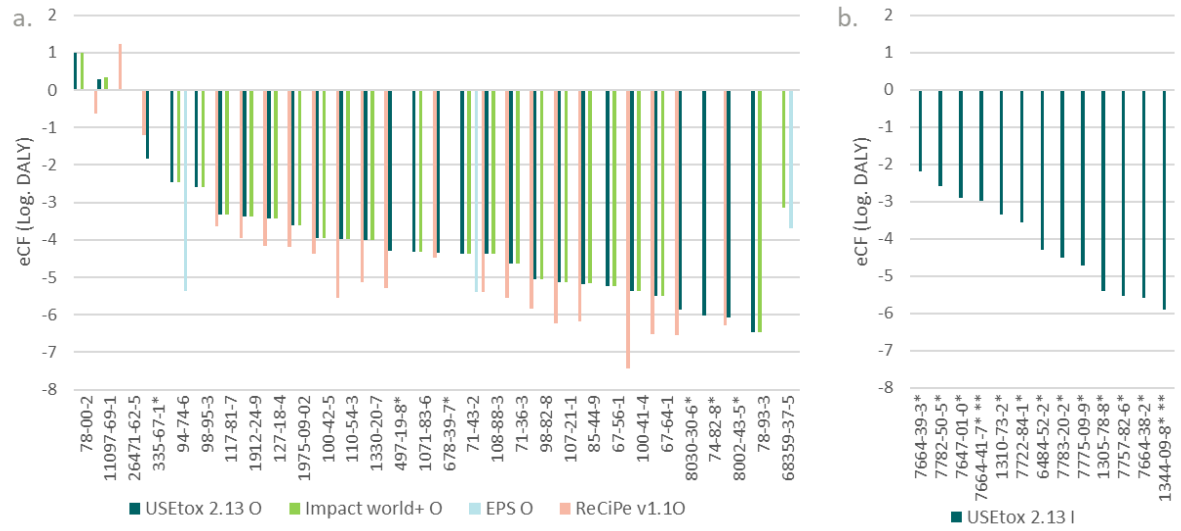

Figure 11. Endpoint, human toxicity – non-cancer CFs (eCFs) from USEtox 2.13, Impact world +, EPS and ReCiPe 2016 v1.1 for the emission compartment air. Sorting based on CFs from/calculated based on USEtox 2.13, high-to-low. Only substances with a CFs are presented in the graphs. CFs calculated as part of this thesis project based on USEtox 2.13 are indicated with an * in connection to the substance's CAS number.

The substances follow a similar pattern for most of the organic substances, with the CFs from USEtox 2.13 and Impact world + being the same or almost the same. The ReCiPe 2016 v1.1 CFs for organic substances differ slightly from those from USEtox 2.13 and Impact world + but still following mainly the same trend when ranking the substances, with some outliers (data points that deviate from the trend). Such outliers, where the CFs from ReCiPe 2016 v1.1 are approximately the same size as the CFs based on USEtox 2.13 are the substances 8:2 FTOH (CAS: 678-39-7) and soybean lecithin (CAS: 8002-43-5). What should be noted is that for both of these substances, the USEtox 2.13 based CFs were calculated as part of this thesis project, which can be a reason for the deviation from the USEtox-ReCiPe relation trend seen for the other CFs from ReCiPe 2016 v1.1. Most of the CFs from ReCiPe are smaller than the ones from USEtox 2.13 and Impact World +, with exception for aroclor 1254 (CAS: 11097-69-1).

Additionally, CFs for three organic substances have been found in EPS. The small number of collected CFs makes it difficult to compare trends between the methods. Although by looking at each substance that has a CF in EPS, which is MCPA (94-74-6), benzene (71-43-2) and cyfluthrin (68359-37-5), MCPA is much lower whereas benzene and cyfluthrin are more similar compared to the USEtox based methods.

For the inorganic substances, CFs were only obtained from USEtox 2.13, and these were all calculated outside of the scope of the method and should only be seen as a test.

3.5.4 Comparison of methods based on monetary assessments

Three of the eight methods assessed were based on monetary valuations: Eco-cost, Environmental prices, and EPS. However, since the valuations in EPS in made based on all environmental impacts considered applicable for a certain substance group and not only toxicity, the monetary valuation of substances in EPS could not be compared with the other methods. The monetary valuation of the non-cancerous human toxicity impacts and

ecotoxicity impacts of the studied substances for Eco-cost and Environmental prices are shown in Figure 12 and Figure 13.

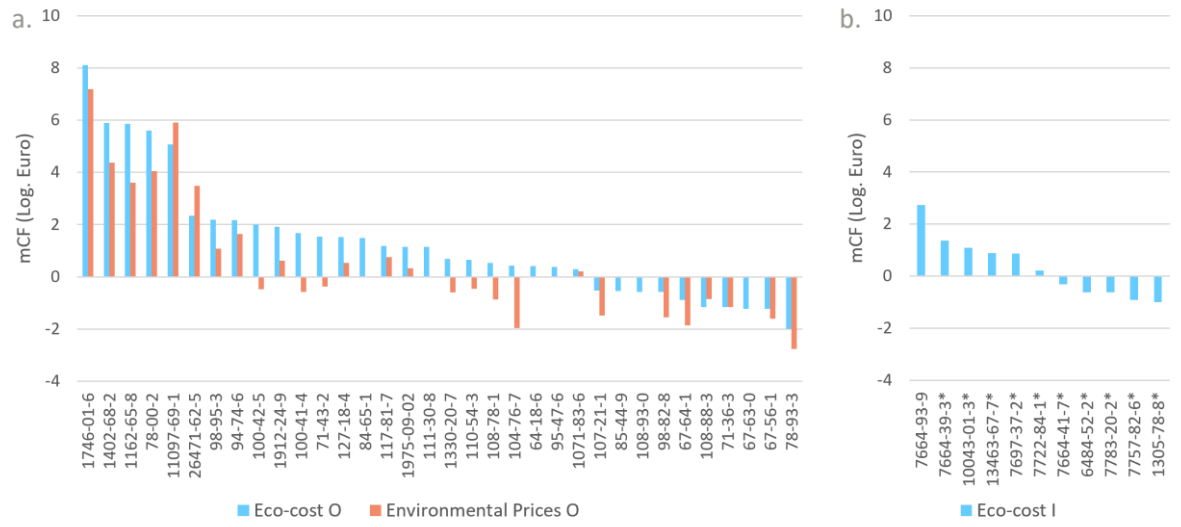

Figure 12. Human toxicity – non-cancer CFs for the monetary LCIA methods Eco-cost and Environmental prices for the emission compartment air. Sorting based on CFs from Eco-cost, high-to-low. Only substances with a CFs are presented in the graphs.

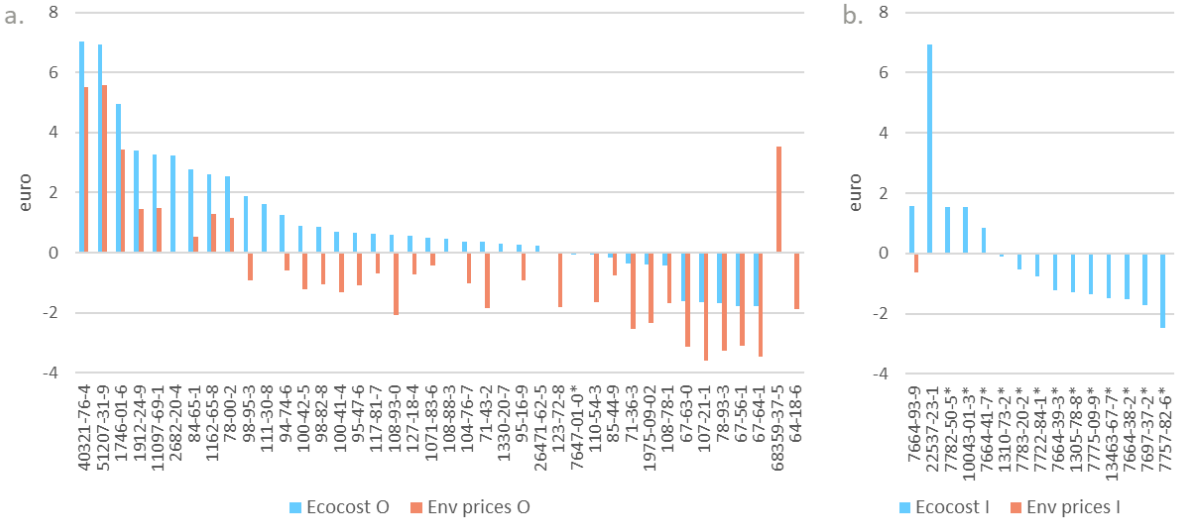

Figure 13. Ecotoxicity CFs for the monetary LCIA methods Eco-cost and Environmental prices for the emission compartment air. Sorting based on CFs from Eco-cost, high-to-low. Only substances with a CFs are presented in the graphs. CFs calculated as part of this thesis project based on USEtox 2.13 are indicated with an * in connection to the substance's CAS number.

As can be observed in the figures, the two methods follow mainly the same trend relating to the ranking order of the different substances. Eco-cost covers both organic and inorganic substances, unlike Environmental prices which covers only organic substances. For most substances, Environmental prices scores are lower compared to those from Eco-cost, with the exception of substances aroclor 1254 (CAS: 11097-69-1) and 2,4/2,6-toluenediisocyanate (CAS: 26471-62-5). The differences between the two methods are due to the use of different methods as basis for the monetary valuation, as well as differences in the assigned monetary valuations of the substances. Eco-cost constitutes of

CFs from EF3.1 paired with a monetary value of 216000 €/CTUh for the human toxicity – non-cancer category, 920000 €/CTUh for the human toxicity – cancer category and 0.00289 €/CTUe for the ecotoxicity category (Sustainability Impact Metrics, n.d.). Environmental prices on the other hand is based on CFs from ReCiPe 2016 v1.1 multiplied with a monetary value of 0.158 €/1,4-dichlorobenzene (de Bruyn et al., 2018).

Using the same approach, a monetary valuation of substances could also be reached using the CFs of other methods as a basis, if only deciding on a monetary value for the unit used in the method. The application of a monetary approach can help make an impact more comprehensible, making it easier to evaluate the impact before making a decision.

3.5.5 Uncertainties with the characterization factors

The CFs vary in reliability. The reliability is affected by multiple factors, like data use, substance group, and conversions or assumptions used during the calculation process. The CFs calculated as a part of this thesis project based on USEtox 2.13 have been indicated to pay attention to which CFs which should be considered more uncertain.

In general, inorganic substances (except for metals) are thinly reported in most methods. Out of the eight methods assessed in the study, only three claim to cover the inorganic substance group: EF3.1, ProScale and EPS. Inorganic substances behave differently than organic substances do, making their movements and fates in the environment harder to predict. For example, inorganic substances in the dataset studied here include salts which dissociate in water. Such dissociating substances have one set of properties when solid, and another set of properties when they dissociate, as they then split into its components, becoming "new" substances.

For the calculations, uncertainties arise from the data handling. Use of predicted data instead of experimental makes the results less reliable since the data then originate from a predictive model instead of something measured in real life. Additionally, the (eco)toxicity data can also be a source of uncertainty, partly by the selection of data points, partly by conversions made to adjust the data to the right format for the model. The data point selection, where the most sensitive, relevant data point should be selected, was challenging to do without prior knowledge in (eco)toxicology. (Eco)toxicity data were also given as different points of departure, where some had to be adjusted before use. Conversion of these data points from one point of departure type to another, or from one test duration to another (acute/sub-chronic/chronic) using a conversion factor introduces uncertainty, since the conversion factor has been made up by other (eco)toxicity data and might not match the data at hand.

3.6 Life cycle assessment results

The total (eco)toxicity impacts at endpoint level using the methods that were included in LCA for Experts (USEtox 2.12, EF3.1 and ReCiPe 2016 v1.1) are shown in Figure 14a-d. A USEtox version to which CFs calculated for this thesis project, based on USEtox 2.13, have been added is also included and indicated with an asterisk (*). Figure 14a shows the ecotoxicity impacts, expressed in the unit PDF, potentially disappeared fraction of species, for USEtox 2.13 and EF3.1 and as relative species loss for ReCiPe 2016 v1.1. Figure 14b-d shows human toxicity impacts, expressed in the unit DALY, disability-adjusted life years. FU = functional unit, which is defined as 1 m^2 PVC sheet for the system studied.

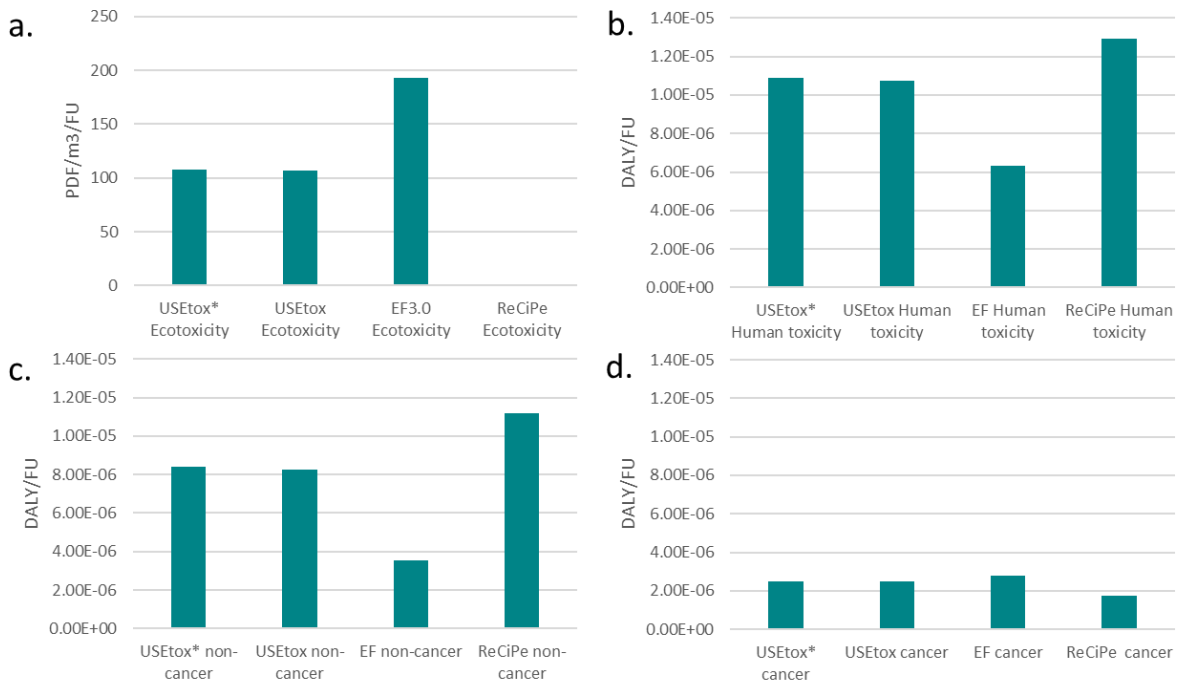

Figure 14. Total: a. ecotoxicity impacts. b. human toxicity impacts (including both cancer and non-cancer effects). c. human toxicity – non-cancer impacts. d. human toxicity – cancer impacts, at endpoint level for the PVC production per functional unit, cradle-to-gate, using the methods USEtox 2.12, EF3.1 and ReCiPe 2016 v1.1. USEtox* is the USEtox 2.12 version in which CFs calculated as part of this thesis project, based on USEtox 2.13, have been added. The ecotoxicity impact from ReCiPe 2016 v1.1 is given in relative species loss, compared to the other methods which present the impact in the unit PDF, potentially disappeared fraction of species. The functional unit is 1m^2 of PVC sheet.

The EF3.1 method is given the highest score in the ecotoxicity category, where the impact score from ReCiPe is not visible at all in the figure since the score is so low. This can be due to a possible difference in units, where USEtox 2.13 and EF3.1 addresses a potentially disappeared fraction of species, while ReCiPe 2016 v1.1 measures the loss of species integrated over time (Huijbregts et al., 2017). The result from ReCiPe says that the loss of species per year, as a consequence of the modelled PVC sheet production, is expected to be low. By converting the units, a more accurate comparison could have been possible. This was however not done in this project due to a lack of time.

The highest impact score in the human toxicity category is achieved by ReCiPe. The chemical footprint from ReCiPe is therefore larger than for the other methods. This follows the trends shown in the comparison of CFs, where the CFs from ReCiPe often took on a higher value than the other methods in the multimedia fate-exposure methods category. A larger population size is also considered in ReCiPe than in USEtox and EF3.1, which can have contributed to the DALY unit being valued differently in the methods, but because lack of time, this has not been confirmed. resulting in different sized footprints. The high score is dominated by non-cancer effects, as the cancer impacts are given low scores in all assessed methods.

The varied sizes of the footprints can also be connected to the extent of data gaps within the methods. If a substance was missing a CF, and it was not possible to calculate and/or add, the toxicity impact of that substance will not have been included in the final chemical footprint. If CFs for many substances were missing in any of the methods, this would have resulted in large uncertainties, possibly presenting a smaller footprint than what is called for. In all impact categories, the two USEtox versions, including or excluding CFs calculated as part of this project, based on USEtox 2.13, are very similar, indicating that the added, calculated CFs did not change the overall impact much.

The results are further decomposed in Figure 15, illustrating a comparison of the total (eco)toxicity impact from the production of 1 m^2 of PVC sheet. The total impact is presented for the three impact categories ecotoxicity, human toxicity - cancer and non-cancer. The graph illustrates the contribution in percentage of potential impact per process step or process category (e.g. transport or energy generation).

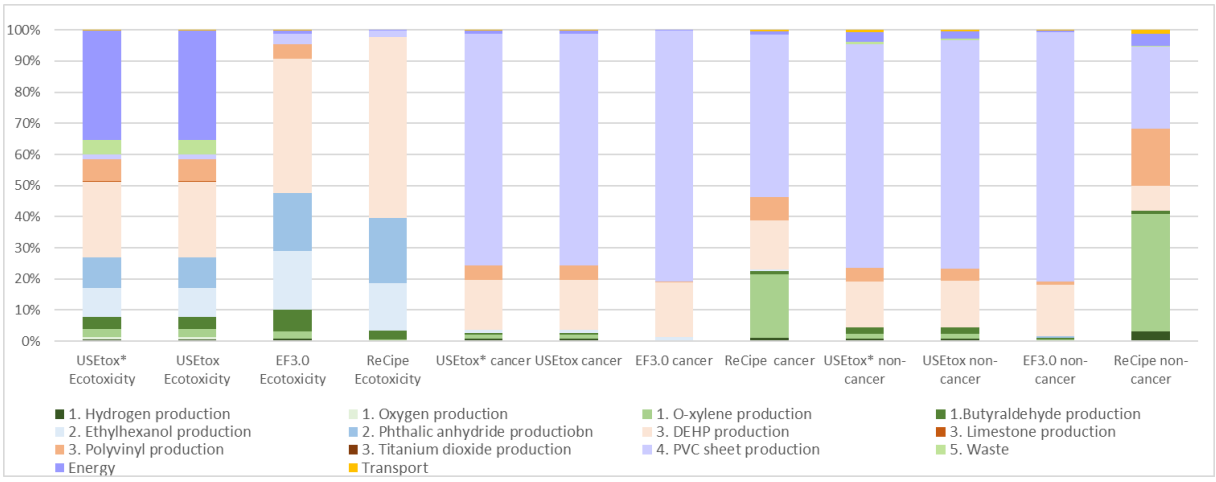

Figure 15. Environmental impact from the different processes in the LCA, using different LCIA methods. USEtox* is the USEtox 2.13 version in which CFs calculated as part of this thesis project, based on USEtox 2.13, have been added. Numbering of methods is according to the grouping in the previously presented flowchart.

For the ecotoxicity category, energy is the process with the largest contribution for both USEtox versions, whereas for both EF3.1 and ReCiPe 2016 v1.1 it is the DEHP production that has the largest impact and almost no contribution from the energy process.

In the impact category human toxicity - cancer, the PVC production has the largest contribution for all the methods. The two USEtox versions and EF3.1 are very similar, except for a smaller contribution from the polyvinyl production in EF. ReCiPe deviates more in this impact category, identifying a larger impact from the o-xylene production. The same pattern can be seen for the non-cancer impact category: USEtox and EF give similar results, whereas ReCiPe deviates even more than from the cancer impact category, as the o-xylene production has an even larger contribution and the polyvinyl production as well.

The categories are further investigated in Table 7, which shows the substances which contribute the most to the total (eco)toxicity impact within the different LCIA methods.

Table 7. Substances which are responsible for more than 10% of the total environmental impact of the PVC sheet production system, using the four LCIA methods available in LCA for Experts. USEtox* is the USEtox 2.13 version in which CFs calculated as part of this thesis project, based on USEtox 2.13, have been added. ET = ecotoxicity, HT-c = human toxicity - cancer, HT-nc = human toxicity – non-cancer.

Impact category	Method	Substances > 10 % of total impact	%	Production process
ET	USEtox 2.12*	Aluminum (Inorganic emissions to fresh water)	18%	Energy
		Iron (Heavy metals to fresh water)	17%	Energy
		Di(2-ethylhexyl)phthalate (DEHP) (Hydrocarbons to fresh water)	11%	DEHP production
	USEtox 2.12	Aluminum (Inorganic emissions to fresh water)	18%	Energy
		Iron (Heavy metals to fresh water)	17%	Energy
	EF3.1	Di(2-ethylhexyl)phthalate (DEHP) (Hydrocarbons to fresh water)	28%	DEHP production
		2-Ethyl-1-hexanol (hydrocarbons to freshwater)	24%	2-Ethylhexanol- and DEHP production
		Xylene (ortho-Xylene; 1.2-Dimethylbenzene) (Hydrocarbons to fresh water)	16%	Phthalic anhydride production
	ReCiPe 2016 v1.1	Di(2-ethylhexyl)phthalate (DEHP) (Hydrocarbons to fresh water)	32%	DEHP production
		Phthalic anhydride (Hydrocarbons to fresh water)	26%	Phthalic anhydride- and DEHP production
		2-Ethyl-1-hexanol (Hydrocarbons to fresh water)	24%	2-Ethylhexanol- and DEHP production
HT-c	USEtox 2.12*	Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	87%	DEHP production and PVC sheet production
	USEtox 2.12	Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	87%	DEHP production and PVC sheet production
	EF3.1	Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	93%	PVC sheet production and DEHP production
	ReCipe v1.1 2016	Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	52%	PVC sheet production
		Chromium (+VI) (Heavy metals to fresh water)	20%	O-xylene production

HT-nc	USEtox 2.12*	Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	84%	PVC sheet production and DEHP production
	USEtox 2.12	Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	91%	PVC sheet production and DEHP production
	EF3.1	Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	91%	PVC sheet production and DEHP production
	ReCiPe v.1.1 2016	Zinc (Heavy metals to fresh water)	33%	O-xylene production
		Di(2-ethylhexyl)phthalate (DEHP) (Halogenated organic emissions to air)	26%	PVC sheet production

It can be observed that the emissions with the most impact in the ecotoxicity category are all emissions to water. The modelled emissions from the DEHP, 2-ethylhexanol and phthalic anhydride productions were major contributing emissions for all methods. These are processes that were modelled as part of the project since they were not included in LCA for Experts. Because of this, these processes are not aggregated, but have been modelled using ERCs for worst-case scenario of emissions. Additionally, for the two USEtox versions, energy is also a major contributing process, because of its emissions of metals. This originates from the energy processes being aggregated processes.

In the impact category human toxicity – cancer, emissions of DEHP are the dominating cause of toxicity impact. Here, the emissions are instead to the air compartment. Only in ReCiPe 2016 v1.1 is another emission identified as also contributing more than 10% to the impact of the process. There, emissions of chromium (+VI) to water are coming from the production of o-xylene, corresponding to 20% of the total cancerous human toxicity impact from the PVC sheet production.

Finally, the human toxicity – non-cancer category is also dominated by emissions of DEHP to air. Again, ReCiPe 2016 v1.1 identifies emissions of heavy metals to water as well as major contributors from the processes, but this time for zinc.

Except for a few metals, the (eco)toxicity impact of the PVC sheet production is dominated by emissions of different carbon compounds. The prominent substances are DEHP, 2-ethylhexanol and phthalic anhydride, which are all processes that were created as a part of the system modelling in LCA for Experts, and therefore had emissions added to them according to ERCs which describe the worst-case scenario emissions. Because of this, it is possible that the emissions were assigned to be bigger than what they would realistically be if the production was put into use and are likely to be higher than other direct emissions as included in the LCA database.

4 Discussion

In this chapter, the results from the assessment of the methods and the LCA system are discussed in relation to the research questions. The methods covered were: USEtox, ProScale, EPS, EF3.1, Impact world+, ReCiPe v1.1 2016, Eco-cost and Environmental Prices

4.1 Ease-of-use and accessibility

The methods for chemical footprint calculations varied in complexity, with some being easier-to-use at the knowledge level of the testers, being engineering students in their final year at university. Gathering of predefined CFs from the methods was easy, provided that the substance searched for was included in the database. For the methods for which calculations were possible, their complexity was connected to how much data were needed for the input parameters, how difficult they were to find and how much data processing that was required. It was also connected to the extent of their instructions and the calculation tool used. A manual where a step-by-step guidance was presented was perceived as easier to follow than an article on the method. Some methods' calculation procedures were described in multiple documents, which were not always coherent or did not provide all needed information in the same document. A single, consistent manual would have been preferred.

Calculations were made in USEtox 2.13, EF3.1 and ProScale, out of which USEtox 2.13 and EF3.1 needed the input data for 11 parameters to calculate a CF, in comparison with ProScale which needed input data for five parameters. While USEtox 2.13 and EF3.1 required the same parameters to be filled in (as EF3.1 originates from USEtox), the data collection strategies differ between the methods. In EF3.1, data should be collected from European databases, making use of data reported from industries/companies within the EU under e.g. REACH and CLP.

ProScale also makes use of reported industry data under REACH, but using fewer parameters (for the impact assessment part, which is what was tested here). This makes the model less complex and easier to use without expert knowledge, demanding only data on H-phrases, vapor pressure (if a fluid) or dustiness (if solid) of each substance to get a score. However, to take the results further, by making a full LCA, other factors need to also be considered. Such factors are MFs, PHFs and PROCs for the full system model. The inclusion of these needs more data on the system and its processes, so making a full LCA using ProScale needs in principle an as extensive LCI as the other methods. Today this can be even more challenging to derive in ProScale compared to other approaches as the database with process descriptions still is limited in coverage.

For a substance which is already listed in the ProScale Excel tool (latest update for the "H-phrases-database" sheet in March 2016), the H-phrases are automatically gathered from a database, diminishing the need for gathering data on those, further simplifying the data collection. Data on vapor pressure is easily accessible for most fluid substances, while dustiness is not something that is usually categorized. To assess the dustiness of a solid was challenging to do only using the information provided in the ProScale manual. This assessment would be difficult to do for a person without expert knowledge on solid

materials and their properties, or a laboratory with possibility to test the dustiness level of substances.

For USEtox 2.13 and EF3.1, the parameters that were the most difficult to gather and understand were the (eco)toxicity parameters avlog$_{EC50}$ and ED_{50}. For these parameters, (eco)toxicity data were gathered and had to be processed before use. Selection of (eco)toxicity test data points and conversions of these were difficult to do coming from a more technical background with limited knowledge on the (eco)toxicological field. From the 95th-percentile analysis made in section 3.5.1.1, there is an indication that the (eco)toxicity effect data made a big impact on the toxicity ranking of the substance. This conclusion is also reached by von Borries et al. (2023). This shows the importance of assessing the effect data correctly to get a reliable result. In ProScale this assessment is avoided through the use of H-phrases, for which the toxicity data have already been assessed and classified according to CLP.

4.1.1 Result presentation output

The result output also affects how easy the methods are to use for chemical footprint calculations, since it needs to be presented in a way that is easy to understand and interpret for further use. This depends on both the output format and the unit of the CFs.

The units differ between the methods and are not always easy to understand or compare. The units are not always intuitive, which makes it hard to have a perception of the size of the expected toxicity. For example, a unit that could be more understandable is the use of cases/kg for midpoint level human toxicity effects in USEtox 2.13, EF3.1 and Impact world +. A case of illness is more comprehensible than, for instance, the unit for the same toxicity category in ReCiPe 2016 v1.1, which is given in kg 1,4-DCB. This unit can be less intuitive for understanding the magnitude of a given toxicity score, since it is harder to have a perception on what a kg 1,4-DCB really means. The same could be said for ProScale, in which the results are given as a ProScale score which also does not give any implications on the toxicity level when assessing the score on its own and not in comparison to other substances or systems scores.

At an endpoint level, the challenge of different units remains, but there is also a struggle since some results are converted to the same endpoint unit, but these are based off different things. For example, the DALY unit used by the non-monetary multimedia fate-exposure methods is based on different population sizes in USEtox 2.13 and EF3.1 compared to ReCiPe 2016 v1.1. This makes the methods difficult to compare directly to one another. Then, the monetary methods which give a monetary value as an output could be more comprehensible since money is something that everyone has a perception of and a relationship to. Hauschild and Huijbregts (2015) discuss the presentation of results in LCIA at either midpoint or endpoint level, indicating that endpoint results could be easier to interpret but also highlighting that midpoint level results have a stronger scientific robustness to them.

4.2 Differences between model structures

The model structures varied, based on differences in exposure pathway as well as the consideration of actual impacts, in comparison to predicted impacts.

4.2.1 Direct and indirect exposure

In USEtox version 2.13, which is the version that was used in this report, direct exposure is not assessed. Direct exposure has been included in USEtox version 3.0 beta 6c, referred to as near-field modelling, but this version was not tested during this thesis project. Fantke et al. (2021) stated that direct exposure contributes more to a life cycle assessment when comparing direct and indirect exposure based on case studies but since the USEtox version 3.0 was not assessed, it is out of this report's scope to understand to what extent the near-field exposure differs from the far-field exposure. Considering Fantke et al.'s statement this could result in an underestimation of the potential (eco)toxicity impact by excluding direct exposure. If the direct exposure has a larger potential impact than the indirect exposure, the chemical footprint will at least double and this could be significant in a weighting step, resulting in a larger contribution from toxicity in the total potential environmental impact. However, the inclusion of direct exposure in the LCA results in a weighting step, including also other impact indicators, require careful consideration of implications of the inclusions of effects of emissions still in the Technosphere, something which is normally not included in environmental LCA.

ProScale was the only method assessed in this report that was based on direct exposure. Comparing ProScale with USEtox 2.13 nothing could be said about the size of the potential impact magnitudes as indicated by the CF, instead the CFs pattern was compared. This comparison highlighted substances like for example Naphtha, that attained very different CFs when comparing ProScale and USEtox 2.13. Only assessing indirect exposure, the substance would not be considered that hazardous. However, by not assessing a direct exposure, a significant potential impact could be missed. The same reasoning can used for the opposite case, if only assessing direct exposure substances that are more persistent and have the ability to exist longer in the environment could be undervalued. Both direct and indirect exposure need to be included in an assessment to ensure coverage of all routes of chemical exposure to humans and that all effects are included.

4.2.2 Consideration of actual impacts

A method that also is based on fate-exposure modelling is EPS. The reason for the few CFs found within the EPS method for the 73 substances analyzed in this report is because the method is based only on "actual" impacts, i.e. verified cause-effect chains from environmental measurements (Steen, 1999). The small coverage of substances makes it an inadequate LCIA method when focusing on toxicity assessment specifically. Substances such as PFOA or aflatoxin, that received high CFs in both USEtox and in ProScale are not assessed in EPS. Including actual impacts in an LCIA method could be time-consuming, as each substance must be assessed based on case-specific studies. This is further problematic as there are so many chemicals in use today and the introduction of new chemicals is important to be able to assess before an effect can be identified. Although the

method has disadvantages, its advantage is that it raises the discussion on credibility, as the method is based on real-case scenarios.

4.2.3 Parameter and substance coverage effect on life cycle assessment results

Only three methods were assessed in the LCA and these methods were based on the USEtox method. The result from the LCA showed how small differences between the CFs could have a relatively large impact on the result, regarding which processes that contributes the most to the total impact. These differences in the result are connected to how cause effect chains from emission to impact are foreseen in the different methods, but also which substances have a CF. Looking at the LCA result for ecotoxicity the energy processes had the largest contribution when assessed with USEtox. Iron and aluminum can be found as the two substances with the largest potential impact. According to Gandhi and Diamond (2018) the aluminum CF is overestimated in USEtox 2.1 and this is because of the aspect of speciation, meaning that aluminum can be found in different forms, leading to varying characteristics depending on the aluminum composition. EF3.1 and ReCipe v1.1 did not have iron or aluminum as the main contributor to the potential impact. In the case of EF3.1 this could be connected to the robustness factor, that results in a lower CFs for inorganic substances. Sauter et al. (2020) states that the assessment of metals should proceed with caution considering dissociation and degradation for inorganic substances including metals. For ReCiPe v1.1 no speculations are made on this matter due to limited knowledge on how the model handles metals, although what can be noticed is that the metals chromium and zinc had a large potential impact in the o-xylene production for human toxicity, cancer respective human toxicity, non-cancer.

Variations in model structure leads to different outcomes being in focus. Comparing USEtox with ProScale the discussion of direct and indirect exposure is the most significant aspect when analyzing the CFs. Whereas for the USEtox based methods it is the use of the parameters and substance coverage.

4.2.4 Chemical footprint

The use of USEtox 2.13, EF3.1 and ReCiPe v1.1 in the LCA resulted in a partial chemical footprint, based on the definition in this report. A full chemical footprint would of course require a cradle-to-grave assessment. In addition, direct exposure of humans during manufacturing and use stages were not included. ProScale, EPS, Impact world+, Eco-cost and Environmental prices also had the possibility to generate a chemical footprint, meaning that each methods CFs could have been used to assess the potential impact for the PVC sheet. By using the definition set in this report, including elements of CRA and LCA, the size of the “foot” was assessed, although it says nothing about the resilience of the planet in relation to this footprint. This result can then only be used to compare chemical footprints assessed with the same method or methods that have the same unit, showing that one foot is bigger than the other, although it can be difficult to understand the significance of the issue without a benchmark. Ideally, the capacity of the planet would be considered, meaning the assessment of the chemical footprint could be compared to a limit or a boundary. There are no set planetary boundaries for chemicals, making it difficult to understand how the methods could be used at this time (Rockström et al., 2009; Steffen et al., 2015).

4.3 Area of use

The results from the chemical footprint calculation can be used in different industrial contexts.

4.3.1 Innovation stage

The differences between the methods make them variously well suited for different decision contexts within the industry. At an innovation stage, for a new product, service, or process, it can be useful to use a method which needs minimal work, since a company would not want to invest too much time and money in an alternative which might not end up being used. For this purpose, all methods could be of use if the substances in focus are already included in the method's database. However, in a case where a new substance is invented, this approach does not work since the substance will not be included in the database of any method. Then, depending on which substance group the new substance belongs to, the only options are to use USEtox or EF3.1 to calculate a new CF, or to use a proxy substance. Both USEtox 2.13 and the EF3.1 method work for calculation of organic substances and cationic metals, but if an inorganic substance, only EF3.1 can handle such substances. For both methods, data on the physiochemical properties, fate and toxicity is needed and therefore must be available, estimated, or produced. This data collection and handling process can be time consuming, so at an innovation stage as described above where minimal work ought to be invested, the use of proxy substances could be more efficient.

4.3.2 Purchase scenario

The LCIA methods can also be useful in a purchase scenario. In a situation where a company is buying a substance to use in their production, different aspects, like life cycle potential toxicity impact, can be of importance for their investment decision. Investment in substances with a low toxic impact potential reported during their lifecycle can be important to the company, to be able to later report a small chemical footprint of their product, process, or service to their consumers. To achieve this, it is important that suppliers can provide data on the chemical footprint of their production, including the whole lifecycle of the product, so that it is later possible to get the full picture of its (eco)toxicity impacts. The challenge with this reporting system is to make sure that all suppliers use data of the correct type and quality, and that the results that are provided are equal and comparable, so that it can later be used by consumers when comparing products and deciding which to buy. This correct and equal reporting can be demanding for smaller companies which might not have the expertise needed in both the LCA and toxicity field.

4.3.3 Communication

When used for communication, it is important that the chemical footprint results are easy to understand and interpret. Depending on the audience, what is perceived as clear communication can vary. Without prior knowledge on chemical footprints, understanding a CF or an impact score from an LCA can be hard, depending on the units as discussed before. In these cases, when trying to communicate an impact to consumers, the monetary methods can be an alternative since money is something everyone have a relationship with, making it possible to comprehend the differences between different options easier. The same can be said about the unit DALY, disability-adjusted life years, which communicates impacted years of life which people also can have a perception of. Presentation of results in other units which are less intuitive for an average consumer,

like for example kg 1,4 DCB eq. or ProScale scores, can be more relevant in a business-to-business scenario.

However, communication of results from an LCA comes with some requirements. According to the ISO 14040 standard, LCA results that will be used for comparison have to be critically reviewed by a third party (Baumann & Tillman, 2004).

4.4 Intended operator of the chemical footprint calculation methods

As described above, the methods for chemical footprint calculations can be useful in different industrial contexts, and careful method selection is needed to achieve relevant results. In addition to the relevance of a method in relation to its use context, the ease-of-use can depend on who is the intended user of the method. Coming from a more technical background but with knowledge on LCA, the toxicity data handling in USEtox 2.13 and EF3.1 can be challenging to do in a correct way. Then, a structure like the one in ProScale, where the toxicity data have already been assessed and classified by a professional in toxicology can be simpler to use. However, the opposite could be said for ProScale, where the toxicity data handling has been simplified, but an element of LCA is needed, connecting an LCI to the use of the substances in the process. This can instead be a struggle for people coming from a background in the toxicology field.

4.5 Recommendations for future development

Based on the insights given by this project, some things have been considered as important for future work on LCIA methods for chemical footprint calculations. We highlight the following important aspects:

- Inclusion of both direct and indirect exposure, depending on the safeguard subject under study
    - Direct exposure is of importance for humans, while indirect exposure to a substance can affect both humans and ecosystems
- Simplification of (eco)toxicity data handling
    - The selection of (eco)toxicity data points was found challenging without having in-depth knowledge on toxicology. A structure like the one in ProScale where the toxicity assessment has already been made by a professional and classified using hazard phrases would be preferred.
- Need for a pedagogical calculation tool, in which it is clear where to enter data, where the results are given and no manual adjustments to the equations need to be made.
- Use of a unit which is comprehensible and comparable.
- The potential to implement the method in an LCA.
    - This is based on the model structure, units of the assessed potential impact and if it makes the method implementable in the traditional workflow for an LCA, as set by the ISO14040 standard. For example, ProScale which does not result in traditional CFs, makes the resulting scores hard to use when performing the last step of the LCA process where a comparison between units and impact categories is to be made.

5 Conclusions

The LCIA methods for chemical footprint calculations could be categorized based on their accessibility (referring to their substance coverage), potential to calculate new CFs, their capability to be used in LCA software and the presentation of the potential impact (if the result is comprehensive and easy to understand). If new CFs could be calculated then these calculations differed in ease-of-use, considering aspects such as the instructions and tools for calculating the CFs and the number of parameters required. The difficulty in collection and handling of data for the required parameters varied between methods. For example, the collection of (eco)toxicity effect data was considered difficult for the USEtox based methods in comparison with the collection of H-phrases used in ProScale. The latter was preferred by the writers of this report, being engineering students in their final year. The data collection could also differ in data sources used.

The methods were also categorized into two categories, one based on fate-exposure modelling, including a sub-category for, monetary valuation, and one with scoring based on exposure banding. Furthermore, the model structures could be distinguished on the basis of indirect and direct exposure considerations. Exposure pathways are important to consider, as the CFs can differ considerably depending on the method used and there is a risk of missing potential impacts from a substance. For the fate-exposure type of methods assessing indirect exposure, the CFs are more similar between methods. Despite this, small differences can still have significant effects as was seen in the LCA results. Differences in CF relative rank and size can be traced to alterations between parameters and the substance coverage, partly affected by the inclusion or non-inclusion of inorganic substances.

The results from this thesis project could be used as a mapping for industrial users to get a better understanding of how methods differ between each other and for which contexts different methods could be suitable, although no specific recommendation can be given. During the project, the complexity of chemical footprint calculations has been assessed, highlighting the need for knowledge in both the fields of toxicology and of life cycle assessment. When constructing a chemical footprint, it is important to consider that the knowledge level of the user applying the method in both fields can vary. As few people are experts in both LCA and toxicology, the chemical footprint methods need to be easy to use, while also having a model structure that is not over-simplified, which could generate unreliable results. There is currently no one method today that can be considered the best in all aspects and contexts. To find this balance the LCIA methods for chemical footprint calculations must continue to develop.

6 References

Aurisano, N., Albizzati, P. F., Hauschild, M., & Fantke, P. (2019). Extrapolation Factors for Characterizing Freshwater Ecotoxicity Effects. *Environmental Toxicology and Chemistry*, *38*(11), 2568-2582.

Baitz, M., Byrne, E., Kreissig, J., Frees, N., Bey, N., Hansen, M. S., Hansen, A., Bosch, T., Borghi, V., & Watson, J. (2004). Life Cycle Assessment of PVCand of principal competing materials.

Baumann, H., & Tillman, A.-M. (2004). *The hitch hiker's guide to LCA* (Vol. 1).

Benoît, C., Norris, G. A., Valdivia, S., Ciroth, A., Moberg, A., Bos, U., Prakash, S., Ugaya, C., & Beck, T. (2010). The guidelines for social life cycle assessment of products: just in time! *The International Journal of Life Cycle Assessment*, *15*, 156-163.

Bjørn, A., Diamond, M., Birkved, M., & Hauschild, M. Z. (2014). Chemical Footprint Method for Improved Communication of Freshwater Ecotoxicity Impacts in the Context of Ecological Limits. *Environmental Science & Technology*, *48*(22), 13253-13262.

Bjørn, A., Owsianiak, M., Molin, C., & Laurent, A. (2018). Main characteristics of LCA. *Life cycle assessment: theory and practice*, 9-16.

Boguski, T. K. (2006). Understanding Units of Measurement. *Environmental Science and Technology Briefs for Citizens*, (2), 2.

Brack, W., Ait-Aissa, S., Backhaus, T., Birk, S., Barceló, D., Burgess, R., Cousins, I., Dulio, V., Escher, B. I., Focks, A., van Gils, J., Ginebreda, A., Hering, D., Hewitt, L. M., Hilscherová, K., Hollender, J., Hollert, H., Köck, M., Kortenkamp, A., . . . Altenburger, R. (2019). Strengthen the European collaborative environmental research to meet European policy goals for achieving a sustainable, non-toxic environment. *Environmental Sciences Europe*, *31*(1), 63.

Brack, W., Escher, B. I., Müller, E., Schmitt-Jansen, M., Schulze, T., Slobodnik, J., & Hollert, H. (2018). Towards a holistic and solution-oriented monitoring of chemical status of European water bodies: how to support the EU strategy for a non-toxic environment? *Environ Sci Eur*, *30*(1), 33.

Bulle, C., Margni, M., Patouillard, L., Boulay, A.-M., Bourgault, G., De Bruille, V., Cao, V., Hauschild, M., Henderson, A., Humbert, S., Kashef-Haghighi, S., Kounina, A., Laurent, A., Levasseur, A., Liard, G., Rosenbaum, R. K., Roy, P.-O., Shaked, S., Fantke, P., & Jolliet, O. (2019). IMPACT World+: a globally regionalized life cycle impact assessment method. *The International Journal of Life Cycle Assessment*, *24*(9), 1653-1674.

Caldeira, C., Garmendia Aguirre, I., Tosches, D., Mancini, L., Abbate, E., Farcal, R., Lipsa, D., Rasmussen, K., Rauscher, H., Riego Sintes, J., & Sala, S. (2023). *Safe and Sustainable by Design chemicals and materials - Application of the SSbD framework to case studies* (JRC131878). P. O. o. t. E. Union.

Campos, K. R., Coleman, P. J., Alvarez, J. C., Dreher, S. D., Garbaccio, R. M., Terrett, N. K., Tillyer, R. D., Truppo, M. D., & Parmee, E. R. (2019). The importance of synthetic chemistry in the pharmaceutical industry. *Science*, *363*(6424), eaat0805.

de Bruyn, S., Bijleveld, M., de Graaff, L., Schep, E., Schroten, A., Vergeer, R., & Ahdour, S. (2018). *Environmental Prices Handbook, EU28 version*.

de Simone Souza, H. H., de Abreu Evangelista, P. P., Medeiros, D. L., Albertí, J., Fullana-i-Palmer, P., Boncz, M. Á., Kiperstok, A., & Gonçalves, J. P. (2021). Functional unit influence on building life cycle assessment. *The International Journal of Life Cycle Assessment*, *26*, 435-454.

Diamond, M. L., de Wit, C. A., Molander, S., Scheringer, M., Backhaus, T., Lohmann, R., Arvidsson, R., Bergman, Å., Hauschild, M., & Holoubek, I. (2015). Exploring the planetary boundary for chemical pollution. *Environment International*, *78*, 8-15.

Guidance on information requirements and chemical safety assessment, Chapter R.12: Use descriptor system, (2009).

Guidance on information requirements and chemical safety assessment, Chapter R.16: Environmental exposure assessment, (2016).

Erhart, S., & Erhart, K. (2022). Application of North European characterisation factors, population density and distance-to-coast grid data for refreshing the Swedish human toxicity and ecotoxicity footprint analysis. *Environmental Impact Assessment Review*, *92*, 106686.

Fantke, P., Chiu, W. A., Aylward, L., Judson, R., Huang, L., Jang, S., Gouin, T., Rhomberg, L., Aurisano, N., McKone, T., & Jolliet, O. (2021). Exposure and Toxicity Characterization of Chemical Emissions and Chemicals in Products: Global Recommendations and Implementation in USEtox. *Int J Life Cycle Assess*, *26*(5), 899-915.

Fantke, P., & Ernstoff, A. (2018). LCA of Chemicals and Chemical Products. In M. Z. Hauschild, R. K. Rosenbaum, & S. I. Olsen (Eds.), *Life cycle assessment: theory and practice* (pp. 783-815). Springer International Publishing.

Fantke, P., Huijbregts, M. A. J., van de Meent, D., Margni, M., Jolliet, O., Rosenbaum, R. K., McKone, T. E., & Hauschild, M. (2015d). *USEtox® 2.0 Manual: Organic Substances (Version 2)*.

Frontera, P., Salieri, B., & Righi, S. (2020). Comparison of the LCIA methods used for the evaluation of chemicals. *Life Cycle Assessment in the Chemical Product Chain: Challenges, Methodological Approaches and Applications*, 33-51.

Gandhi, N., & Diamond, M. L. (2018). Freshwater ecotoxicity characterization factors for aluminum. *The International Journal of Life Cycle Assessment*, *23*, 2137-2149.

Gust, K. A., Collier, Z. A., Mayo, M. L., Stanley, J. K., Gong, P., & Chappell, M. A. (2016). Limitations of toxicity characterization in life cycle assessment: Can adverse outcome pathways provide a new foundation? *Integrated environmental assessment and management*, *12*(3), 580-590.

Hauschild, M., McKone, T., van de Meent, D., Huijbregts, M. A. J., Margni, M., Rosenbaum, R. K., Jolliet, O., & Fantke, P. (2017).

Hauschild, M. Z., & Huijbregts, M. A. J. (2015). Introducing Life Cycle Impact Assessment. In M. Z. Hauschild & M. A. J. Huijbregts (Eds.), *Life Cycle Impact Assessment* (pp. 1-16). Springer Netherlands.

Hitchcock, K., Panko, J., & Scott, P. (2012). Incorporating chemical footprint reporting into social responsibility reporting. *Integrated Environmental Assessment & Management*, *8*(2).

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. (2017). ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. *The International Journal of Life Cycle Assessment*, *22*(2), 138-147.

Jacquemin, L., Pontalier, P.-Y., & Sablayrolles, C. (2012). Life cycle assessment (LCA) applied to the process industry: a review. *The International Journal of Life Cycle Assessment*, *17*, 1028-1041.

Leclerc, A., Sala, S., Secchi, M., & Laurent, A. (2019). Building national emission inventories of toxic pollutants in Europe. *Environment International*, *130*, 104785.

Lexén, J., Belleza, E., Loh Lindholm, C., Rydberg, T., Amann, N., Aschford, P., Bednarz, A., Coërs, P., Dornan, P., & Downes, R. (2021). ProScale-A life cycle oriented method to assess toxicological potentials of product systems (2017): Guidance Document version 1.5. In.

Margni, M., Rossier, D., Crettaz, P., & Jolliet, O. (2002). Life cycle impact assessment of pesticides on human health and ecosystems. *Agriculture, Ecosystems & Environment*, *93*(1), 379-392.

Muralikrishna, I. V., & Manickam, V. (2017). Chapter Five - Life Cycle Assessment. In I. V. Muralikrishna & V. Manickam (Eds.), *Environmental Management: Science and Engineering for Industry* (pp. 57-75). Butterworth-Heinemann.

Naidu, R., Biswas, B., Willett, I. R., Cribb, J., Kumar Singh, B., Paul Nathanail, C., Coulon, F., Semple, K. T., Jones, K. C., Barclay, A., & Aitken, R. J. (2021). Chemical pollution: A growing peril and potential catastrophic risk to humanity. *Environment International*, *156*, 106616.

Nordborg, M., Arvidsson, R., Finnveden, G., Cederberg, C., Sörme, L., Palm, V., Stamyr, K., & Molander, S. (2017). Updated indicators of Swedish national human toxicity and ecotoxicity footprints using USEtox 2.01. *Environmental Impact Assessment Review*, *62*, 110-114.

Pryshlakivsky, J., & Searcy, C. (2021). Life Cycle Assessment as a decision-making tool: Practitioner and managerial considerations. *Journal of Cleaner Production*, *309*, 127344.

Rockström, J., Steffen, W., Noone, K., Persson, Å., Chapin, F. S., Lambin, E. F., Lenton, T. M., Scheffer, M., Folke, C., Schellnhuber, H. J., Nykvist, B., de Wit, C. A., Hughes, T., van der Leeuw, S., Rodhe, H., Sörlin, S., Snyder, P. K., Costanza, R., Svedin, U., . . . Foley, J. A. (2009). A safe operating space for humanity. *Nature*, *461*(7263), 472-475.

Rojo, F. (2013). DNA Footprinting. In S. Maloy & K. Hughes (Eds.), *Brenner's Encyclopedia of Genetics (Second Edition)* (pp. 360-363). Academic Press.

Rosenbaum, R. K., Bachmann, T. M., Gold, L. S., Huijbregts, M. A. J., Jolliet, O., Juraske, R., Koehler, A., Larsen, H. F., MacLeod, M., Margni, M., McKone, T. E., Payet, J., Schuhmacher, M., van de Meent, D., & Hauschild, M. Z. (2008). USEtox—the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. *The International Journal of Life Cycle Assessment*, *13*(7), 532-546.

Rydberg, T., Sala, S., Bjørn, A., Molander, S., Payet, J., Posthuma, L., Sörme, L., Vighi, M., & Zijp, M. C. (2014). Towards a common conceptual framework for chemical footprint bridging Risk Assessment and Life Cycle Assessment: Short review and way forward. SETAC Europe Annual Meeting, Basel, (CH).

Saavedra-Rubio, K., Thonemann, N., Crenna, E., Lemoine, B., Caliandro, P., & Laurent, A. (2022). Stepwise guidance for data collection in the life cycle inventory (LCI) phase: Building technology-related LCI blocks. *Journal of Cleaner Production*, *366*, 132903.

Sala, S., & Goralczyk, M. (2013). Chemical footprint: A methodological framework for bridging life cycle assessment and planetary boundaries for chemical pollution. *Integrated environmental assessment and management*, *9*(4), 623-632.

Sala, S., Wolf, M.-A., & Pant, R. (2012). *Characterisation factors of the ILCD Recommended Life Cycle Impact Assessment methods. Database and supporting information*.

Saouter, E., Biganzoli, F., Ceriani, L., Versteeg, D., Crenna, E., Zampori, L., Sala, S., & Pant, R. (2018). *Environmental footprint: update of life cycle impact assessment*

methods-ecotoxicity freshwater, human toxicity cancer, and non-cancer. Publications Office of the European Union.
Steen, B. (1999). *A systematic approach to environmental priority strategies in product development (EPS): version 2000-general system characteristics*. Citeseer.
Steen, B. (2019). *Monetary valuation of environmental impacts: Models and data*. CRC Press.
Steffen, W., Richardson, K., Rockström, J., Cornell, S. E., Fetzer, I., Bennett, E. M., Biggs, R., Carpenter, S. R., De Vries, W., De Wit, C. A., Folke, C., Gerten, D., Heinke, J., Mace, G. M., Persson, L. M., Ramanathan, V., Reyers, B., & Sörlin, S. (2015). Planetary boundaries: Guiding human development on a changing planet [Article]. *Science*, *347*(6223), Article 1259855.
Sustainability Impact Metrics. (n.d.). *The concept, structure, and midpoint tables of the eco-costs for LCA*.
Sörme, L., Palm, V., & Finnveden, G. (2016). Using E-PRTR data on point source emissions to air and water—First steps towards a national chemical footprint. *Environmental Impact Assessment Review*, *56*, 102-112.
Tamaru, K. (1991). The history of the development of ammonia synthesis. In *Catalytic Ammonia Synthesis: Fundamentals and Practice* (pp. 1-18). Springer.
Tarasova, N., & Makarova, A. (2016). Assessment of the chemical pollution in the context of the planetary boundaries. *Russian Chemical Bulletin*, *65*, 1383-1394.
Tarasova, N. P., Makarova, A. S., Vinokurov, S. F., Kuznetsov, V. A., & Shlyakhov, P. I. (2018). Green chemistry and sustainable development: approaches to chemical footprint analysis. *Pure and Applied Chemistry*, *90*(1), 143-155.
Technical Committee ISO/TC 207, E. M. (2006). *Environmental management-life cycle assessment-principles and framework*. International Organization for Standardization.
United Nations Environment Programme. (2019). *Global Chemicals Outlook II*
United States Environmental Protection Agency. (2012). *Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11*. In United States Environmental Protection Agency.
United States Environmental Protection Agency. (2021). ToxValDB v9.4. In.
Vanham, D., Leip, A., Galli, A., Kastner, T., Bruckner, M., Uwizeye, A., van Dijk, K., Ercin, E., Dalin, C., Brandão, M., Bastianoni, S., Fang, K., Leach, A., Chapagain, A., Van der Velde, M., Sala, S., Pant, R., Mancini, L., Monforti-Ferrario, F., . . . Hoekstra, A. Y. (2019). Environmental footprint family to address local to planetary sustainability and deliver on the SDGs. *Science of The Total Environment*, *693*, 133642.
von Borries, K., Holmquist, H., Kosnik, M., Beckwith, K. V., Jolliet, O., Goodman, J. M., & Fantke, P. (2023). Potential for Machine Learning to Address Data Gaps in Human Toxicity and Ecotoxicity Characterization. *Environmental Science & Technology*, *57*(46), 18259-18270.
Wang, Z., Walker, G. W., Muir, D. C. G., & Nagatani-Yoshida, K. (2020). Toward a Global Understanding of Chemical Pollution: A First Comprehensive Analysis of National and Regional Chemical Inventories. *Environmental Science & Technology*, *54*(5), 2575-2584.
Westh, T. B., Hauschild, M. Z., Birkved, M., Jørgensen, M. S., Rosenbaum, R. K., & Fantke, P. (2015). The USEtox story: a survey of model developer visions and user requirements. *The International Journal of Life Cycle Assessment*, *20*(2), 299-310.

Wiedmann, T., & Minx, J. (2008). A definition of 'carbon footprint'. *Ecological economics research trends*, *1*(2008), 1-11.
Winder, C., Azzi, R., & Wagner, D. (2005). The development of the globally harmonized system (GHS) of classification and labelling of hazardous chemicals. *Journal of hazardous materials*, *125*(1-3), 29-44.
Zijp, M. C., Posthuma, L., & van de Meent, D. (2014). Definition and Applications of a Versatile Chemical Pollution Footprint Methodology. *Environmental Science & Technology*, *48*(18), 10588-10597.

7 Appendix A

Table 8. List of the articles reviewed for the literature review on the chemical footprint concept, with title and author/-s included. Listed alphabetically based on the authors.

Title	Author(-s)
Chemical Footprint Method for Improved Communication of Freshwater Ecotoxicity Impacts in the Context of Ecological Limits	Bjørn et al. (2014)
Towards a holistic and solution-oriented monitoring of chemical status of European water bodies: how to support the EU strategy for a non-toxic environment?	Brack et al. (2018)
Strengthen the European collaborative environmental research to meet European policy goals for achieving a sustainable, non-toxic environment	Brack et al. (2019)
Application of North European characterisation factors, population density and distance-to-coast grid data for refreshing the Swedish human toxicity and ecotoxicity footprint analysis	Erhart and Erhart (2022)
INCORPORATING CHEMICAL FOOTPRINT REPORTING INTO SOCIAL RESPONSIBILITY REPORTING	Hitchcock et al. (2012)
Building national emission inventories of toxic pollutants in Europe	Leclerc et al. (2019)
Updated indicators of Swedish national human toxicity and ecotoxicity footprints using USEtox 2.01	Nordborg et al. (2017)
Towards a common conceptual framework for chemical footprint bridging Risk Assessment and Life Cycle Assessment: Short review and way forward	Rydberg et al. (2014)
Chemical Footprint: A Methodological Framework for Bridging Life Cycle Assessment and Planetary Boundaries for Chemical Pollution	Sala and Goralczyk (2013)
Using E-PRTR data on point source emissions to air and water—First steps towards a national chemical footprint	Sörme et al. (2016)
Assessment of the chemical pollution in the context of the planetary boundaries	Tarasova and Makarova (2016)
Green chemistry and sustainable development: approaches to chemical footprint analysis	Tarasova et al. (2018)
Environmental footprint family to address local to planetary sustainability and deliver on the SDGs	Vanham et al. (2019)

Definition and Applications of a Versatile Chemical Pollution Footprint Methodology	Zijp et al. (2014)

Table 9. List of substances studied, their CAS number and if they were calculated as part of this thesis project based on USEtox 2.13 and EF3.1. If the substances which were not calculated were flagged as indicative in the USEtox 2.01 database is also included. ET = flagged as indicative in the ecotoxicity category, HT = flagged as indicative in the human toxicity category.
*Substances with the three highest CFs in the categories ecotoxicity, human toxicity – cancer and human toxicity – non-cancer.

Substance	CAS number	Calculated as part of this thesis project based on USEtox 2.13	Flagged as indicative in USEtox 2.01 database	Calculated as part of this thesis project based on EF3.1
1,2,3,7,8-PENTACHLORODIBENZO-P-DIOXIN *	40321-76-4		ET	
2,3,7,8-TetraCDD *	1746-01-6		ET	
2,3,7,8-TetraCDF *	51207-31-9		ET	
2,4/2,6-TOLUENEDIISOCYANATE*	26471-62-5		HT	
2-ethylhexanol	104-76-7			
8:2 FTOH	678-39-7	x		x
acetone, liquid	67-64-1			
AFLATOXIN *	1402-68-2			x
Aflatoxin B1 *	1162-65-8		ET	
aluminium sulphate, powder	10043-01-3	x		
Aluminum (|||)	22537-23-1		ET	
ammonia, anhydrous, liquid	7664-41-7	x		x
ammonium nitrate	6484-52-2	x		
ammonium sulphate	7783-20-2	x		
Anthraquinone	84-65-1			
AROCLOR 1254 *	11097-69-1		ET, HT	
Atrazine	1912-24-9			
benzene	71-43-2			
Benzoethiazol	95-16-9		ET	
Butanol	71-36-3			
Butyraldehyde	123-72-8			
calcium chloride	10035-04-8	x		x
chlorine, liquid	7782-50-5	x		
cumene	98-82-8			
cyclohexanol	108-93-0			
Cyflutrin	68359-37-5			
DEHP	117-81-7			
dichloromethane	9/2/1975			
ESBO	8013-07-8	x		x
ethyl benzene	100-41-4			
ethylene glycol	107-21-1			
Formic acid	64-18-6		ET	
Glutaraldehyde	111-30-8			

Glyfosate	1071-83-6		HT	
hexane	110-54-3			
hydrochloric acid, without water, in 30% solution state	7647-01-0	x		
Hydrogen (g) & (l)	1333-74-0	x		x
hydrogen fluoride	7664-39-3	x		
Hydrogen peroxide	7722-84-1	x		
isopropanol	67-63-0			
MCPA	94-74-6		ET, HT	
Melamine	108-78-1			
Methane	74-82-8	x		
methanol	67-56-1			
methyl ethyl ketone	78-93-3		ET	
MIT (Methylisothiazolinone)	2682-20-4			
Naphtha	8030-30-6	x		x
nitric acid, without water, in 50% solution state	7697-37-2	x		
nitrobenzene	98-95-3			
nitrogen, liquid	7727-37-9	x		x
oxygen, liquid	7782-44-7	x		x
o-xylene	95-47-6			
PFOA	335-67-1	x		x
PFOS	1763-23-1	x		x
phosphoric acid, industrial grade, without water, in 85% solution state	7664-38-2	x		
Phthalic anhydride	85-44-9		ET	
quicklime, milled, loose	1305-78-8	x		
soda ash, light, crystalline, heptahydrate	497-19-8	x		
sodium chlorate, powder	7775-09-9	x		
Sodium hydroxide (solution state)	1310-73-2	x		
sodium silicate, spray powder, 80%	1344-09-8	x		x
sodium sulphate, anhydrite	7757-82-6	x		
Soybean lecithin	8002-43-5	x		x
Soybean meal	68308-36-1	x		x
Soybean oil	8001-22-7	x		x
styrene	100-42-5			
sulfuric acid	7664-93-9		ET	
sulphate	14808-79-8	x		
tetrachloroethylene	127-18-4			
Tetraethyl lead *	78-00-2		ET, HT	
titanium dioxide	13463-67-7	x		
toluene, liquid	108-88-3			
xylene	1330-20-7			

Table 10. Description of parameters used for calculations in USEtox 2.13 (Fantke et al., 2017).

Parameter	Description
MW	Molar Weight
pKa ChemClass	pKa chemical class
pKa.gain	pKa base reaction
pKa.loss	pKa acid reaction
K_{OW}	Partitioning coefficient between n-octanol and water
P_{vap25}	Vapour pressure at 25°C
Sol_{25}	Water solubility at 25°C
k_{degA}, k_{degW}, k_{degSl}, k_{degSd}	Degradation rate in air, water, soil, or sediment
$avlog_{EC50}$	Effect concentration
$ED_{50, ing, non-cancer}$ or $ED_{50, inh, non-cancer}$	Human equivalent lifetime dose per person that causes a non-cancer disease probability of 50% after ingestion or inhalation
$ED_{50, ing, cancer}$ or $ED_{50, inh, cancer}$	Human equivalent lifetime dose per person that causes a cancer disease probability of 50% after ingestion or inhalation
BAF_{fish}	Bioaccumulation factor in fish

Table 11. Toxicity data harmonization for USEtox 2.13. MEG = Magnetoencephalography, LEL = Lowest Effect Level, IDLH = Immediately Dangerous to Life or Health, RfC = Reference Concentration.

Category	Headline in the toxicity-database	Description
Test status	qc_status	Only passed tests were used. Failed tests were filtered out.
Numeric qualifier	toxval_numeric_qualifier	1. Test values with the numeric qualifier = were prioritised. For cancer data used for human toxicity calculations, only values with the numeric qualifier = were used.

		2. If no, or insufficient, data were available for that qualifier, values with the qualifiers =< and >= were used. 3. Again, if no, or insufficient, data were available for those qualifiers, values with the qualifiers < and > were used.
Study time	study_duration_value	1. If sufficient data were available, tests with no or negative time registered were disregarded. 2. If insufficient data available, tests with no or negative time registered in this category were considered according to the study type reported in the study duration class category (acute/sub-chronic/chronic).
Dose	toxval_numeric, toxval_numeric_original	Two dose value categories were downloaded with the toxicity data. In case the values in the categories differed, the dose in the category toxval_numeric was used.
Study duration	-	In accordance with the USEtox manual (Fantke et al., 2015c), chronic tests were prioritized, followed by subchronic and lastly subacute or acute tests. Study duration times for classifying a study as chronic/subchronic/subscute/acute (human toxicity) or chronic/acute (ecotoxicity) were given in the USEtox 2.0 manual. • For human toxicity, the study duration time classification was the same for all species: • Acute (<14 days), subacute ((14-28 days), subchronic (29-210 days), and chronic (>210 days) • For ecotoxicity, the study duration time classification depended on species group, with the threshold for chronic studies being: • 12 h for algae 12 h for bacteria 24 h for unicellular animals 72 h for crustaceans

		336 h for molluscs, worms, etc. 720 h for fish The study classification was made manually for human toxicity, and automatically in the USEtox 2.13 tool for ecotoxicity. If enough data were available at a chronic level, acute data were not considered.
Point of departure	toxval_type	In accordance with the USEtox manual (Fantke et al., 2015c), priority was given to chronic ED_{50}/EC_{50}, followed by NOAEL/NOAEC and last LOAEL/LOAEC. If no, or not enough, ED_{50}/EC_{50} data, NOAEL/NOAEC was used. If no, or not enough, NOAEL/NOAEC data, then LOAEL/LOAEC was used. However, in the USEtox 2.13 tool it is also possible to use LD_{50} and TC_{50}, but since those are derived from acute tests, they were only used in case of no other data available. No recommendations for how to prioritize LD_{50} or TC_{50} values were given in the USEtox manual. Other points of departure were disregarded. Examples of such points of departure are MEG, LEL, IDLH and RfC.
Units	toxval_units	For human toxicity calculations of ED_{50} values, mg/m3, mg/kg-day or ppm were considered units. For ecotoxicity calculations of $avlog_{EC50}$, only tests with the unit mg/L were used.
Exposure route	exposure_route	For human toxicity calculations of ED_{50} values, only the two exposure routes oral and inhalation were considered. Other routes like *in vitro*, injection or dermal were disregarded.
Water compartment	exposure_method	For ecotoxicity calculations of $avlog_{EC50}$, only freshwater species

		were considered since freshwater is the scope for USEtox. If not sufficient freshwater data, saltwater species were considered to fill the data gap. Tests made in culture were disregarded.
Endpoint selection	critical_effect	For ecotoxicity data, if multiple endpoints were available for one study, the most sensitive endpoint was selected.

8 Appendix B

The LCA was made to further deepen the understanding of how the CFs are used and what impact the use of different LCIA methods make. For this purpose, a small production system for PVC sheets used for flooring was modelled. The system included the production of PVC sheets and its upstream processes, as well as a waste stream from the PVC sheet production. In the upstream processes, the production of butyraldehyde was included. However, since butyraldehyde was missing in the database used, formaldehyde was used as a proxy. It was assumed to be a similar substance with similar toxic impacts. However, it was later discovered that the upstream productions of the two substances differed greatly, so the use of formaldehyde as a proxy for butyraldehyde was not ideal or as representative as hoped for. But, since the LCA was performed mainly to test out the CFs and get a deepened understanding of the impact of using different LCIA methods, this mistake was accepted and used anyway.

Table 12. LCI for production of butyraldehyde, per kg. Agg. = aggregated process.

Input	Process used in LCA for Experts	Amount	Unit	Comment
Formaldehyde	DE: Formaldehyde (HCHO; 37%) Sphera (agg.)	1,05	kg	Used as a proxy for butyraldehyde
Emissions	Flow used in GaBi	Amount	Unit	Comment
Butyraldehyd to air	n-Butyraldehyde [Group NMVOC to air]	0,05	kg	Based on ERC 1
Butyraldehyd to water	Butyraldehyde (n-; iso-butanal) [Hydrocarbons to fresh water]	0,06	kg	Based on ERC 1
Butyraldehyd to soil	Butyraldehyde [Organic emissions to agricultural soil]	0,0001	kg	Based on ERC 1

Table 13. LCI for Production of 2-ethylhexanol, per kg. Agg. = aggregated process.

Input	Process used in LCA for Experts	Amount	Unit	Comment
Hydrogen	DE: Hydrogen (steam cracker) Sphera (agg.)	0.0382	kg	
Butyraldehyde	Production of butyraldehyde	1.37	kg	Manually added process

Thermal energy	DE: Thermal energy from natural gas (agg.)	5,55	MJ	
Electricity	DE: Electricity grid mix 1kV-60kV Sphera (agg.)	1,11	MJ	
Emissions	Flow used in GaBi	Amount	Unit	Comment
2-Ethylhexanol to air	2-Ethyl-1-hexanol [Group NMVOC to air]	0,05	kg	Based on ERC 1
2-Ethylhexanol to water	2-Ethyl-1-hexanol [Organic emissions to fresh water]	0,06	kg	Based on ERC 1
2-Ethylhexanol to soil	2-Ethyl-1-hexanol [Organic emissions to agricultural soil]	0,0001	kg	Based on ERC 1
Hydrogen to fresh water	Hydrogen [Inorganic emissions to fresh water]	0,00229	kg	Based on ERC 1
Hydrogen to air	Hydrogen [Inorganic emissions to air]	0,00191	kg	Based on ERC 1
Butyraldehyd to air	n-Butyraldehyde [Group NMVOC to air]	0,0685	kg	Based on ERC 1
Butyraldehyd to water	Butyraldehyde (n-; iso-butanal) [Hydrocarbons to fresh water]	0,0822	kg	Based on ERC 1
Butyraldehyd to soil	Butyraldehyde [Organic emissions to agricultural soil]	0,000137	kg	Based on ERC 1

Table 14. LCI for production of phthalic anhydride, per kg. Agg. = aggregated process.

Input	Process used in LCA for Experts	Amount	Unit	Comment
Oxygen (gaseous)	RER: Oxygen (gaseous) Sphera (agg.)	0.38	kg	
O-xylene	RER: o-Xylene PlasticsEurope (agg.)	1,17	kg	

Thermal energy	DE: Thermal energy from natural gas (agg.)	5,55	MJ	
Electricity	DE: Electricity grid mix 1kV-60kV Sphera (agg.)	1.8	MJ	
Emissions	Flow used in GaBi	Amount	Unit	Comment
Oxygen to air	Oxygen [Inorganic emissions to air]	0,0190	kg	Based on ERC 1
Oxygen to water	Oxygen [Inorganic emissions to fresh water]	0,0228	kg	Based on ERC 1
Phthalic anhydride to water	Phthalic anhydride [Hydrocarbons to fresh water]	0,06	kg	Based on ERC 1
Phthalic anhydride to air	Phthalic anhydride [Group NMVOC to air]	0,05	kg	Based on ERC 1
Phthalic anhydride to soil	Phthalic anhydride [Organic emissions to agricultural soil]	0,0001	kg	Based on ERC 1
Xylene to air	Xylene (ortho-Xylene; 1,2-Dimethylbenzene) [Group NMVOC to air]	0,0585	kg	Based on ERC 1
Xylene to water	Xylene (ortho-Xylene; 1,2-Dimethylbenzene) [Hydrocarbons to fresh water]	0,0702	kg	Based on ERC 1
Xylene to soil	Xylene (ortho-Xylene; 1,2-Dimethylbenzene) [Organic emissions to agricultural soil]	0,000117	kg	Based on ERC 1

Table 15. LCI for Production of DEHP, per kg. Agg. = aggregated process.

Input	Process used in LCA for Experts	Amount	Unit	Comment
2-ethylhexanol	Nation: Production of Phtalic anhydride	0.821	kg	Manually added process

Phthalic anhydride	Nation: Production of Phtalic anhydride	0.467	kg	Manually added process
Thermal energy	DE: Thermal energy from heavy fuel oil (agg.)	1,08	MJ	
Transport of 2-ethylhexanol	Transport: 6% RME (agg.)	100	km	Truck, 28-32 tot weight, MPL, 22 t, Euro 6. Transport within Germany.
Transport of phthalic anhydride	Transport: 6% RME (agg.)	100	km	Truck, 28-32 tot weight, MPL, 22 t, Euro 6. Transport within Germany.
Emissions	Flow used in GaBi	Amount	Unit	Comment
2-ethylhexanol to air	2-Ethyl-1-hexanol [Group NMVOC to air]	0,0411	kg	Based on ERC 1
2-ethylhexanol to water	2-Ethyl-1-hexanol [Organic emissions to fresh water]	0,0493	kg	Based on ERC 1
2-ethylhexanol to soil	2-Ethyl-1-hexanol [Organic emissions to agricultural soil]	0.0000521	kg	Based on ERC 1
DEHP to air	Di(2-ethylhexyl)phthalate [Group NMVOC to air]	0,05	kg	Based on ERC 1
DEHP to water	Di(2-ethylhexyl)phthalate [Hydrocarbons to fresh water]	0,06	kg	Based on ERC 1
DEHP to soil	Di(2-ethylhexyl)phthalate [Organic emissions to agricultural soil]	0,0001	kg	Based on ERC 1
Phthalic anhydride to air	Phthalic anhydride [Group NMVOC to air]	0,0234	kg	Based on ERC 1
Phthalic anhydride to water	Phthalic anhydride [Hydrocarbons to fresh water]	0,0280	kg	Based on ERC 1

Phthalic anhydride to soil	Phthalic anhydride [Organic emissions to agricultural soil]	0.00004767	kg	Based on ERC 1

Table 16. LCI for production of PVC sheets, per kg. Agg. = aggregated process.

Input	Process used in LCA for Experts	Amount	Unit	Comment
Polyvinyl chloride granulates (S-PVC)	BE: Polyvinyl chloride granulate (S-PVC) Sphera (agg.)	0.326	kg	
Limestone sand	RER: Limestone, crushed stonefines (Grain size 0/2) (EN15804 A1-A3) Sphera (agg.)	0.588	kg	
DEHP	Nation: Production of DEHP	0.476	kg	Manually added process
Titanium dioxide	Production of titanium dioxide (unit process)	0.0261	kg	
Electricity	SE: Electricity grid mix (agg.)	7.8	MJ	
Transport of DEHP	Transport: 6% RME (agg.)	750	km	Truck, 28-32 tot weight, MPL, 22 t, Euro 6. Transport from Germany to Sweden.
Transport of limestone sand	Transport: 6% RME (agg.)	140	km	Truck, 28-32 tot weight, MPL, 22 t, Euro 6. Transport within Sweden.
Transport of PVC granulates	Transport: 6% RME (agg.)	1300	km	Ship, bulk, coast. Transport from Belgium to Sweden.
Emissions	Flow used in GaBi	Amount	Unit	Comment
DEHP to air	Di(2-ethylhexyl)phthalate	0,357	kg	Based on ERC 3

	[Group NMVOC to air]			
DEHP to water	Di(2-ethylhexyl)phthalate [Hydrocarbons to fresh water]	0,00238	kg	Based on ERC 3
DEHP to soil	Di(2-ethylhexyl)phthalate [Organic emissions to agricultural soil]	0,00119	kg	Based on ERC 3
Titanium dioxide to air	Titanium dioxide [Inorganic emissions to air]	0,0255	kg	Based on ERC 3

Table 17. LCI for incineration of PVC waste, per kg. Agg. = aggregated process.

Input	Process used in LCA for Experts	Amount	Unit	Comment
PVC sheets	SE: PVC in waste incineration plant (agg.)	1	kg	

9 Appendix C

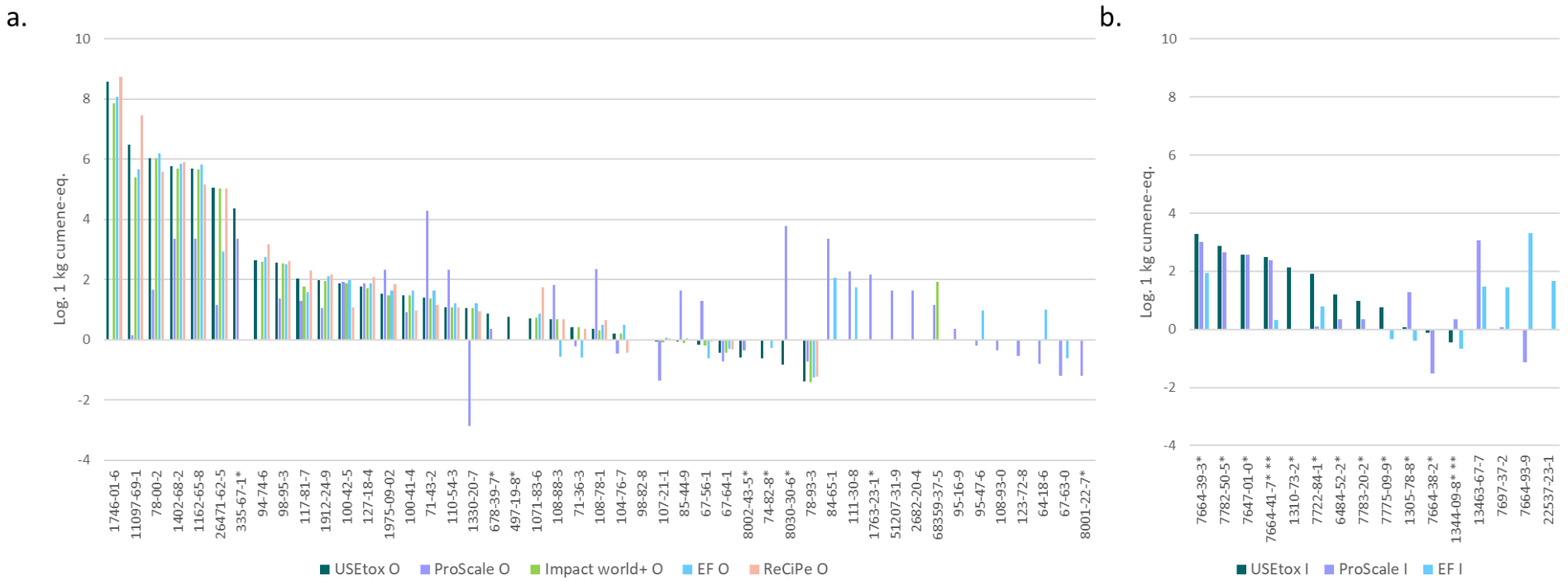

Figure 16 shows the midpoint CFs for the impact category human toxicity, including both cancer and non-cancer and the compartment of emission is air. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following

emission compartments were used for the different methods: USEtox 2.13= Industrial indoor air, ProScale= Industrial air, Impact world+= Indoor air, EF3.1= Indoor air, ReCiPe 2016 v1.1 = Urban air.

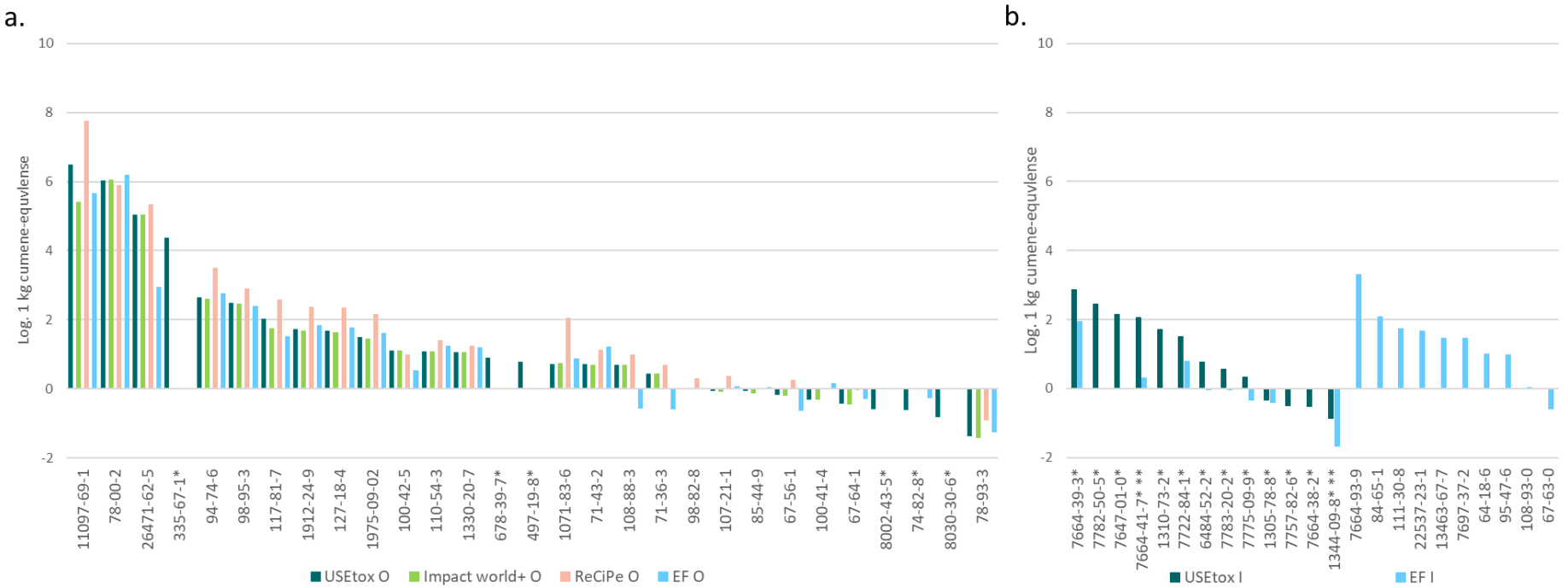

Figure 17 shows the midpoint CFs for the impact category human toxicity, non-cancer and the compartment of emission is air. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= Industrial indoor air, Impact world+= Indoor air, EF3.1= Indoor air, ReCiPe 2016 v1.1 = Urban air.

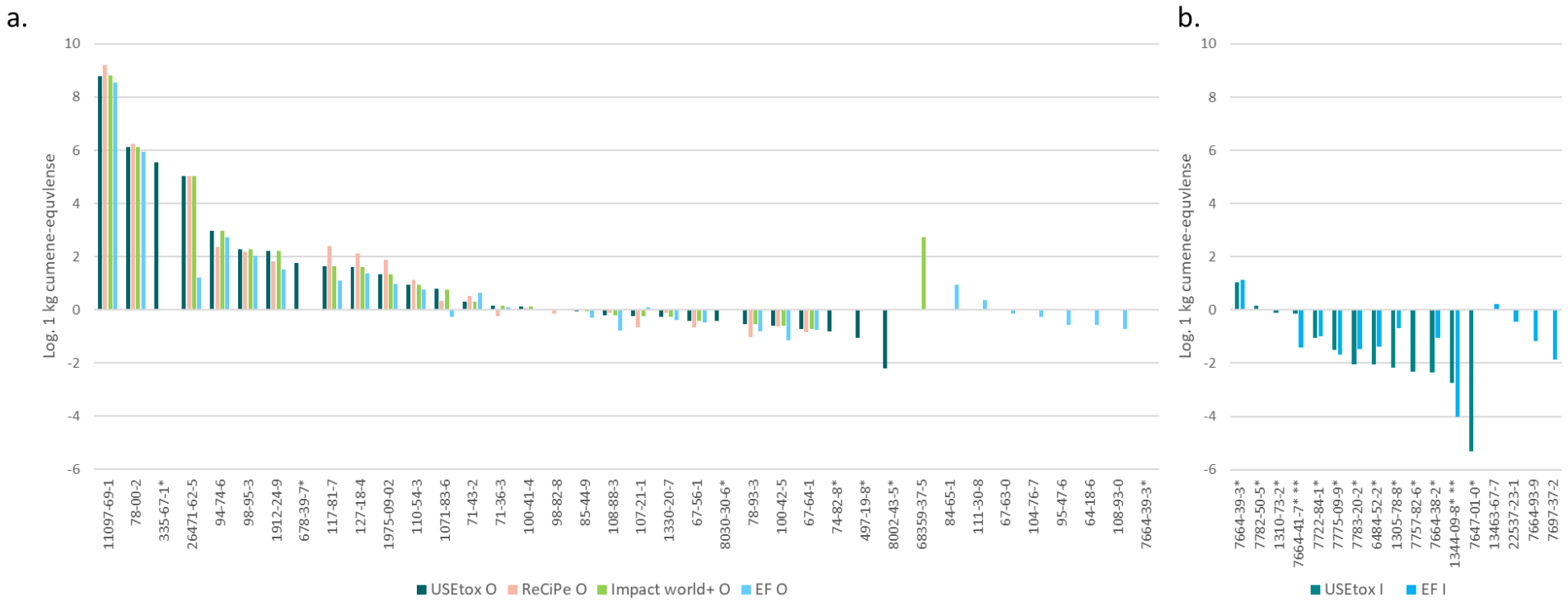

Figure 18 shows the midpoint CFs for the impact category human toxicity, non-cancer and the compartment of emission is water. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= freshwater, Impact world+= lake, EF3.1= freshwater, ReCiPe 2016 v1.1 = freshwater.

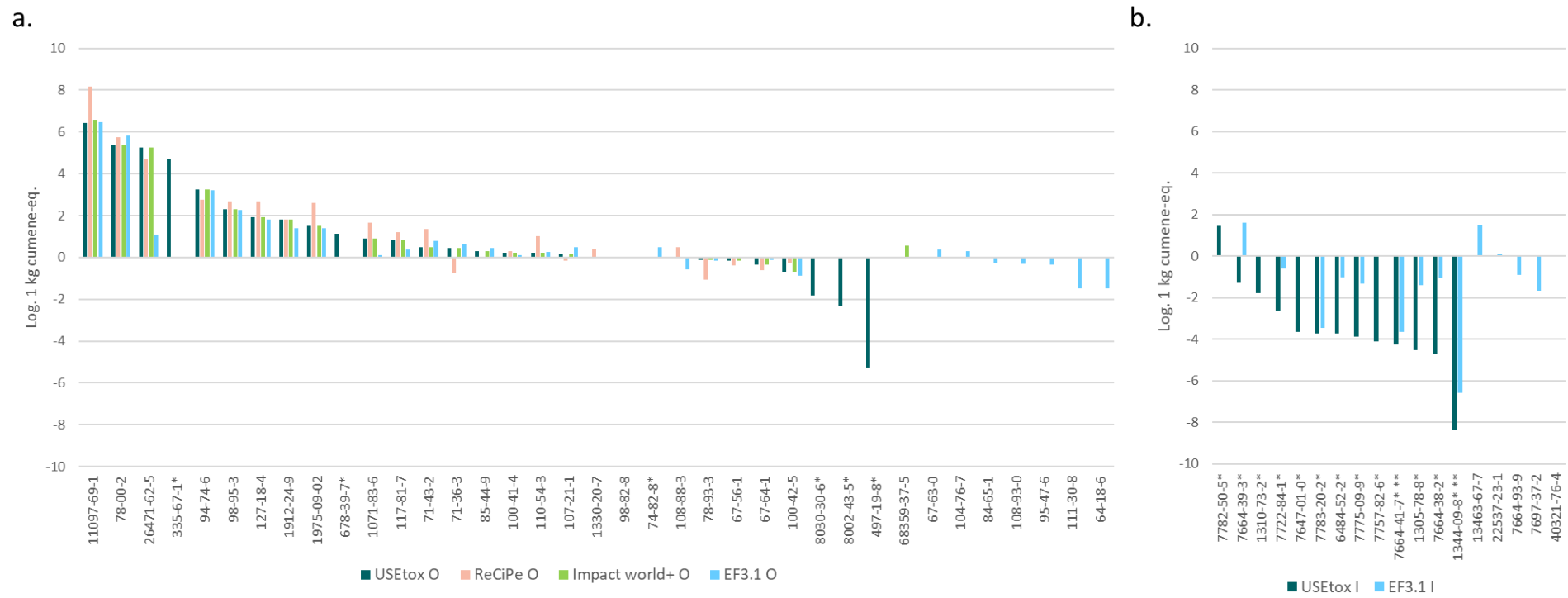

Figure 19 shows the midpoint CFs for the impact category human toxicity, non-cancer and the compartment of emission is soil. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= agricultural soil, Impact world+= agricultural soil EF3.1= agricultural soil, ReCiPe 2016 v1.1 = agricultural soil.

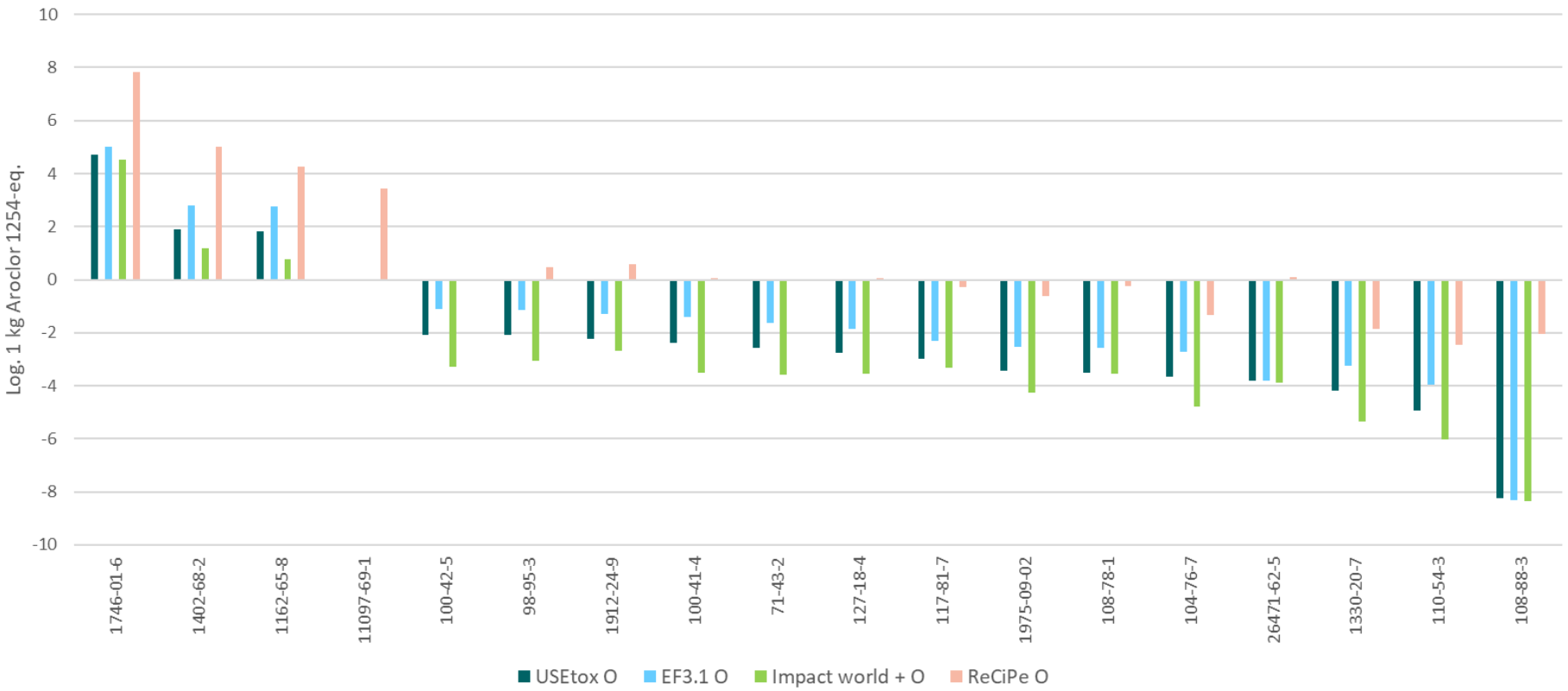

Figure 20 shows the midpoint CFs for the impact category human toxicity, cancer and the compartment of emission is air. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= Industrial indoor air, Impact world+= Indoor air, EF3.1= Indoor air, ReCiPe 2016 v1.1 = Urban air.

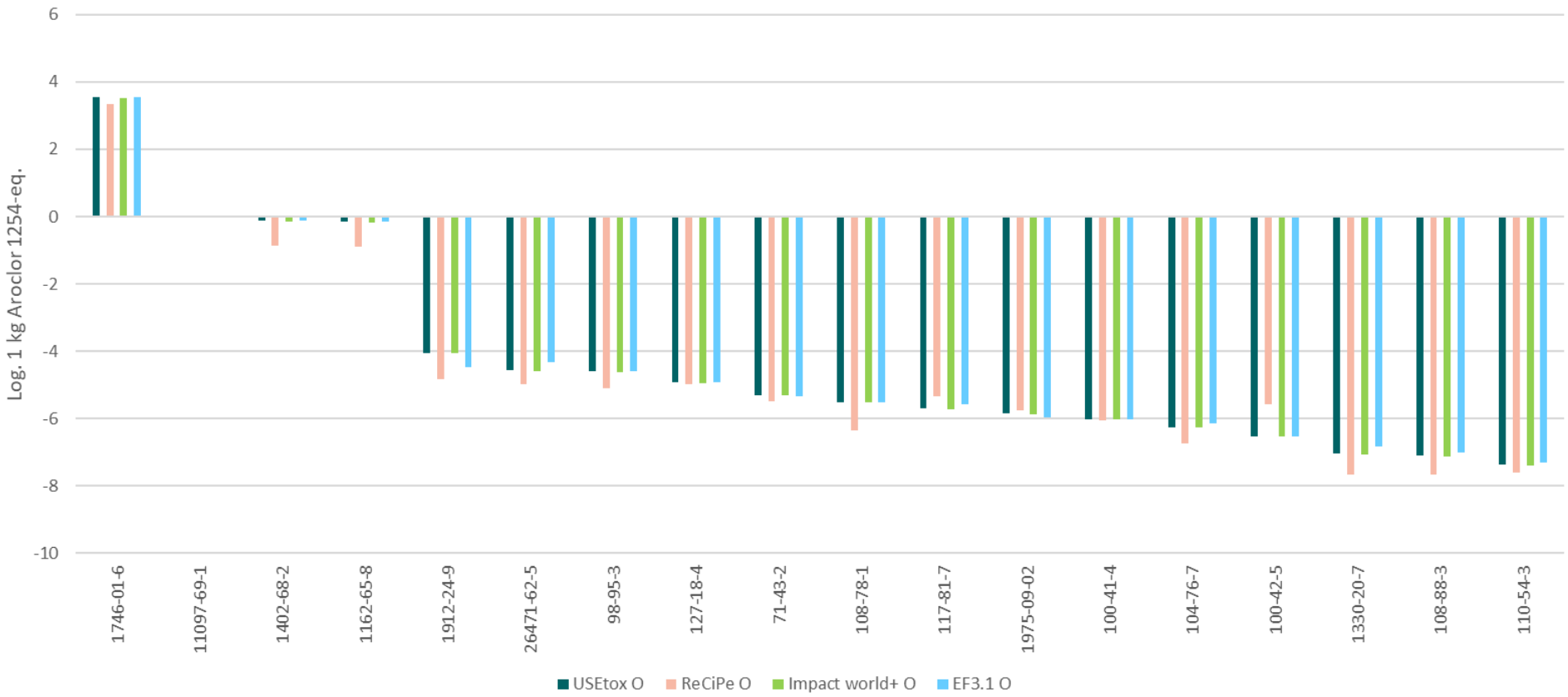

Figure 21 shows the midpoint CFs for the impact category human toxicity, cancer and the compartment of emission is water. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= freshwater, Impact world+= lake, EF3.1= freshwater, ReCiPe 2016 v1.1 = freshwater.

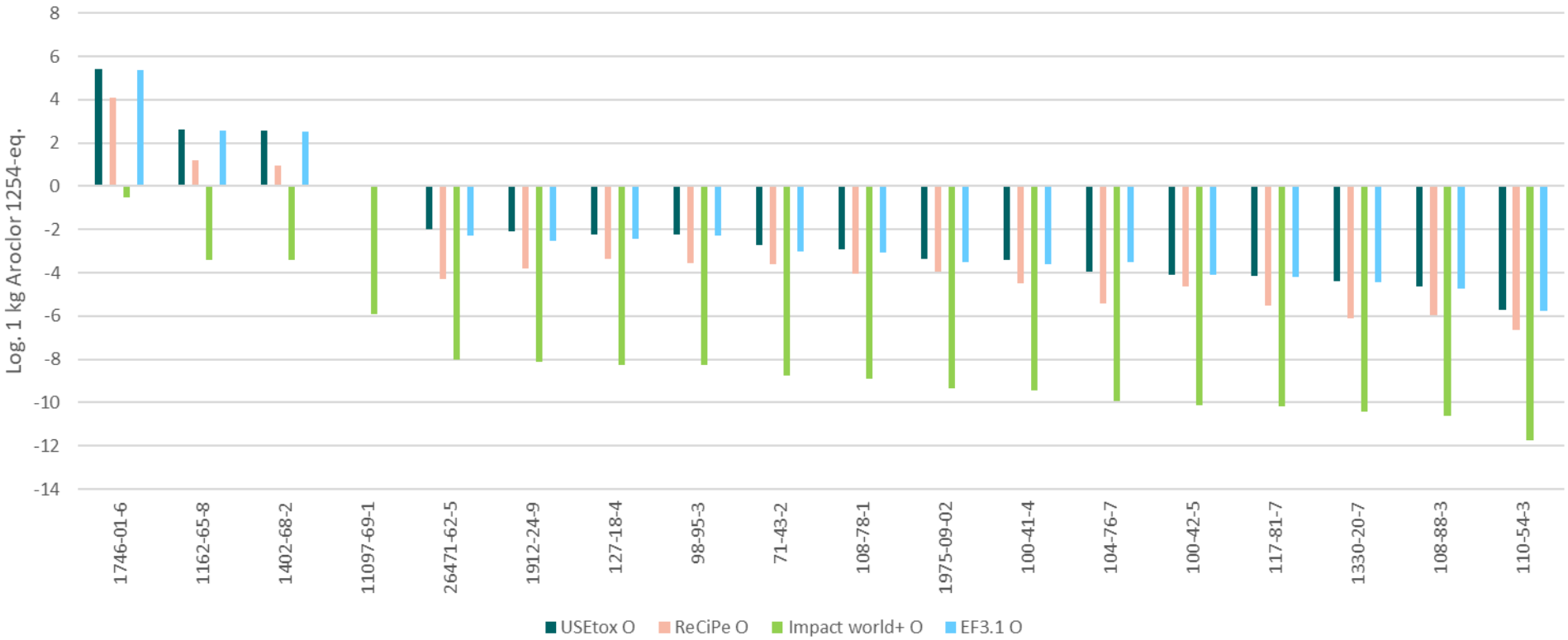

Figure 22 shows the midpoint CFs for the impact category human toxicity, cancer and the compartment of emission is soil. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= agricultural soil, Impact world+= agricultural soil EF3.1= agricultural soil, ReCiPe 2016 v1.1 = agricultural soil.

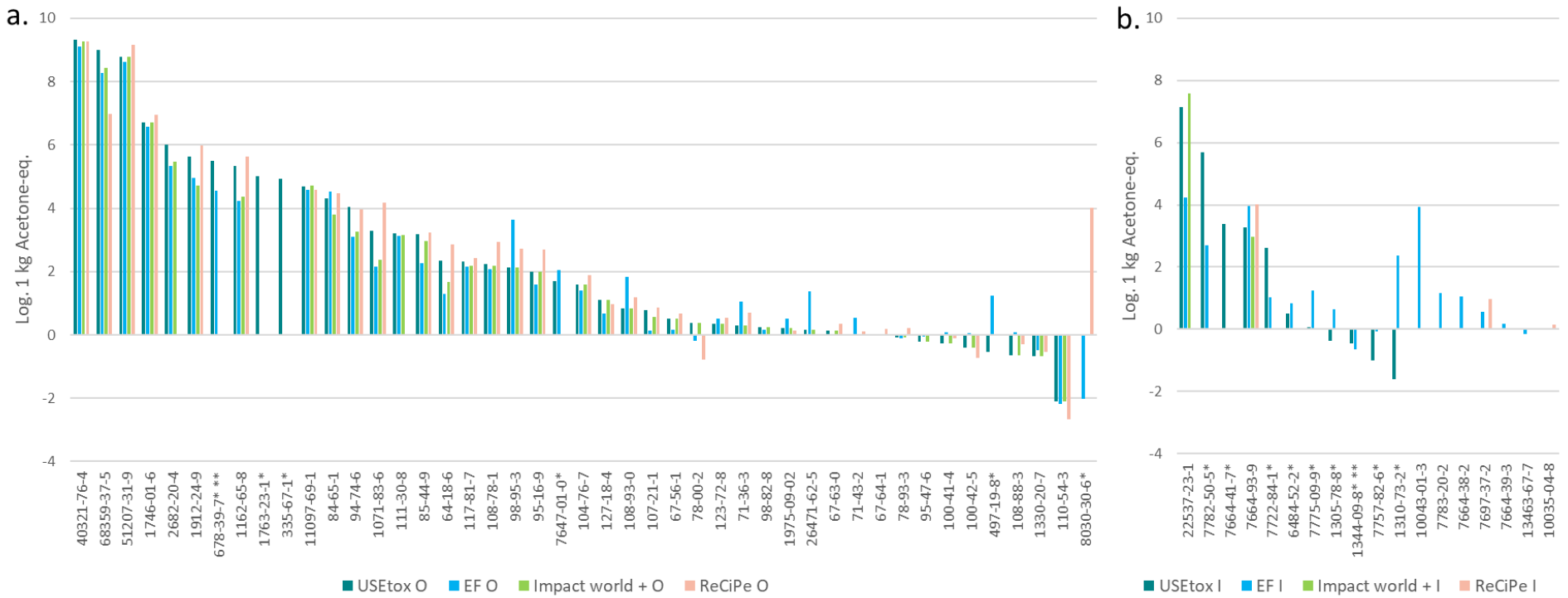

Figure 23 shows the midpoint CFs for the impact category ecotoxicity and the compartment of emission is air. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= urban air, Impact world+= high population air, EF3.1= urban air, ReCiPe 2016 v1.1 = Urban air.

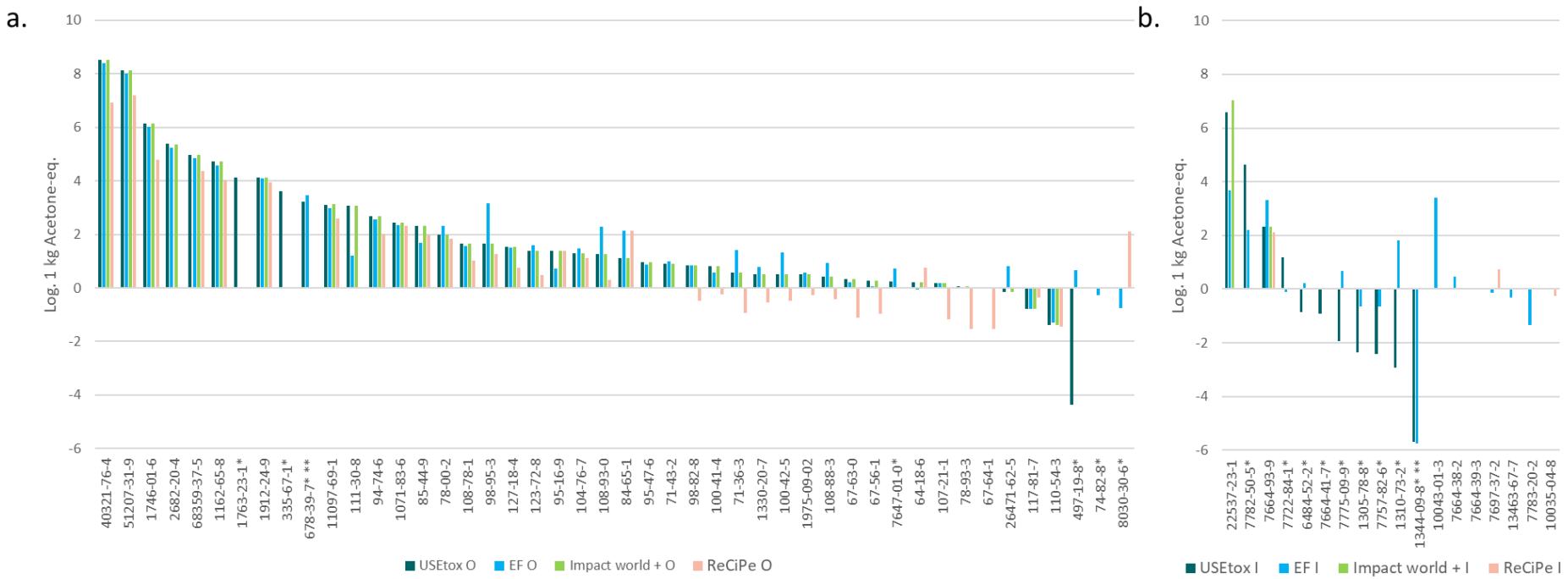

Figure 24 shows the midpoint CFs for the impact category ecotoxicity and the compartment of emission is soil. The graph is on a logarithmic scale and the substances are normalized based on the substance of Cumene. The following emission compartments were used for the different methods: USEtox 2.13= agricultural soil, Impact world+= unspecified soil, EF3.1= agricultural soil, ReCiPe 2016 v1.1 = agricultural soil.

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