ecetoc

Freshwater ecotoxicity as an impact category in life cycle assessment

Technical Report No. 127

Freshwater ecotoxicity as an impact category in life cycle assessment

Technical Report No. 127

ECETOC Technical Report No. 127

Freshwater ecotoxicity as an impact category in life cycle assessment

Contents

SUMMARY

Background. There is an increasing interest to obtain holistic assessments of environmental impact of chemicals, i.e. integrating aspects such as aquatic ecotoxicity, eutrophication, climate change etc. To that end, life cycle assessment (LCA) is seen as key assessment method. The currently ongoing 'Product Environmental Footprint' (PEF) project by the European Commission collects experience in the application of the LCA methodology to the assessment of products. The ultimate objective of this project is to provide LCA-based metrics as a basis for distinguishing between products according to their overall environmental impact. Aquatic ecotoxicity is one of the impacts assessed within LCA. At the same time, there is the understanding that the currently used methodology for environmental risk assessments (ERA) of chemicals is limited with regard to characterising environmental impact of chemicals.

Objectives. The assessment of the risk of adverse effects in the environment originating from the uses and emissions of chemicals is at the heart of ECETOC's activities. Hence, ECETOC established a task force to evaluate the extent to which the limitations of the environmental risk assessment methodology are relevant for the ecotoxicity assessment in LCA, and to identify options for including the ecotoxicity impact of chemicals into assessments of products reflecting their environmental impact in a holistic manner. The following terms of reference guided the work of the task force.

Terms of Reference

1. Conduct a scientific evaluation of the USEtox method, currently the leading method for calculating ecotoxicity impacts in LCA, and its relevance to the real world;
2. Investigate the relationship of USEtox to chemical risk assessment methodology;
3. Provide guidance on the scientific relevance and interpretation of USEtox results in the context of chemical impact assessment and selection of chemical-based (manufactured) products.

Approach

The task force started out with a comparison of the ecological risk assessment versus LCA as predictive approaches for approximating environmental impact of chemicals (Chapter 2). With regard to LCA the focus was put on the ecotoxicity evaluation via the USEtox methodology. This comparison was complemented by another comparison between the USEtox methodology and the 'Critical Dilution Volume'-(CDV) method (Chapter 3). This method is applied for assessing impact of chemical-based products, e.g. in the EU EcoLabel schemes for detergent and personal care products. In addition, Chapter 3 also provides brief outlines of the 'Environmental Safety Check' and the 'ProScale'-method. Beyond the conceptual aspects, this comparison included a case study (Chapters 4 and 5), which highlighted the differences between LCA and CDV regarding the assessment methodology and issues regarding availability and quality of data.

Building on the results of Chapter 2, the USEtox methodology for assessing ecotoxicity is put into the perspective of the greenhouse gas impact assessment in LCA (Chapter 6). This chapter also contains a reflection on the joint report 'New Challenges in Risk Assessment' by the EU Commission's scientific committees on newly identified health risks, on health and environmental risks and on consumer protection.

Finally, Chapter 7 outlines options for proceeding with ecotoxicity in holistic environmental product impact assessment, taking into account the results of the preceding Chapters.

Outcome – Comparison of LCA versus Ecological Risk Assessment

The comparison of the ecological risk assessment versus the freshwater ecotoxicity assessment concluded that both methods (and CDV and ProScale as well) are based on the same type of input information. In addition, the metric is obtained in a very similar manner, i.e. by using single-species ecotoxicity data as a reference point for deriving the impact metric. Similarly, in lower-tier risk assessment and in LCA the exposure assessment assumes that the concentrations do not vary in time and space. Hence, there are large methodological similarities.

However, there are discrepancies regarding the assessment objectives, the scopes of the assessment, and the efficiency strategies applied in the assessment. Ecological risk assessment attempts to demonstrate that ecological impact is unlikely and that no risk management is needed. From that point of view, these assessments typically start with a low initial demand for accuracy and proceed in a tiered fashion. They often start with conservative / worst-case assumptions to avoid false negative conclusions regarding the safe use of a chemical. If needed, a stepwise increase of realism is accomplished by refining the input data or turning to refined / higher tier prediction tools. In contrast, LCA attempts to provide a numerical expression of the ecotoxicity impact. Hence, the ambition is to be realistic. The ecotoxicity assessment in LCA addresses the emissions originating from the entire life cycle of a product or a service and hence addresses a multitude of chemicals. Chemical risk assessment typically considers the single use or a single life cycle step of a single chemical.

The major efficiency strategy in risk assessment is to take a tiered approach to increasing the realism of the assessment. This allows to invest the minimum of effort needed for demonstrating that the predicted environmental concentrations do not exceed the effect thresholds. Hence, ecological risk assessments can have a very low to a very high degree of realism. In order to solve the practical difficulty to obtain the large amount of data required to assess all the emissions along the entire life-cycle, so-called life cycle inventories are an essential element for applying LCAs. The life cycle inventories contain the emissions of individual life cycle steps. The emissions along the entire life cycle are obtained as the sum of the emissions, which for many life cycle steps are obtained from the life cycle inventories.

We describe several mechanisms by which uncertainties are introduced into the impact assessment stage of an LCA. These can be due to uncertainties in the characterisation factors or missing characterisation factors. Additionally, differences in granularity and perspective of the datasets in LCI databases can give rise to apparent differences in impact size. However, these data gaps and differences in granularity are not obvious and can at present only be found by tedious analysis.

Outcome - Case studies

In the case study a virtual product consisting of several chemicals is assessed. Disposal of the product via wastewater is part of the life cycle. This disposal scenario represents a worst-case for aquatic ecotoxicity and can also be covered by the CDV method. According to the LCA assessment results obtained with USEtox, impact of the disposal of the product to the wastewater is at least orders of magnitude larger than that of the

earlier life cycle stages. This indicates that the earlier life cycle stages may be negligible for assessing the impact of products which are disposed of via wastewater. The results of the CDV assessments are poorly correlated to those of the assessment with USEtox with regard to the ranking and the absolute scores of the constituents of the product in the scope of our case study. Differences in results obtained with USEtox and CDV are based on differences in the models, but are also due to the data used in the parametrization of either model.

For assessment of the impact of the disposal stage in LCA with USEtox and for the CDV assessment, the input data set is amended in order to obtain a complete set of characterisation factors. These summarise the ecotoxicological properties such as degradability, partitioning behaviour and ecotoxicity. The LCA of the earlier life-cycle stages has to rely on the database data. Closer analysis of these data reveals that characterisation factors for potentially relevant substances are missing. This lack of data is not easily visible in current LCA practice and requires a tedious manual analysis of the results. As a consequence, the LCA assessor cannot know the quality of the LCA result without checking the quality of the database data.

Outcome - Putting LCA into perspective

The comparison of the greenhouse gas assessment with the ecotoxicity assessment in LCA indicates that the latter is much more complex and suggests that the result of the ecotoxicity assessment is significantly less certain than that of the greenhouse gas assessment. The aspect of the uncertainty of the ecotoxicity assessment is followed up by considering the degree of realism of the ecological risk assessment. This is relevant given the methodological similarities between the ecotoxicity assessments in LCA and ecological risk assessment given that the LCA ecotoxicology assessment bears much resemblance to an initial tier environmental risk assessment of a mixture of chemicals. According to the scientific committees of the EU commission (Scientific Committee on Consumer Safety – SCENIHR; Scientific Committee on Health and Environmental Risks - SCHER; Scientific Committee on Consumer Safety - SCCS), the methodology underlying ecological risk assessment is sufficiently conservative for identifying ecological risks. However, it is too uncertain to provide a realistic characterisation of the impact of chemicals on the aquatic environment. In summary, it is concluded that the ecotoxicological assessment methodology is unsuitable for characterising the actual environmental impact because of large uncertainties in results. In consequence, these may not be a valid basis for distinguishing products from each other based on the real environmental impact.

Addressing Ecotoxicity for Comparing Products / Services - Possible ways forward

Nevertheless, there is a considerable demand for comprehensive evaluations of the environmental impact of products and services. Hence, the task force developed options for addressing this need in the future. These options are intended as a basis for a discussion for a multi-stakeholder discussion, e.g. in a joint workshop of the EU Commission, independent experts, and participants of the EU product environmental footprint project.

Within these options, there are two options addressing ecotoxicity without the result being reflected in the LCA assessment. Four additional options consider ecotoxicity as an integral part of life cycle assessment. The most obvious (and the most difficult to implement) option is to improve the ecological risk assessment methodology and subsequently the LCA methodology that would be based on it. The target is to achieve a degree of certainty enabling the size of the ecotoxicological impact of one product to be compared to that of another product. A second option is to make use of the abundance of REACH data in the current USEtox

methodology in order to increase the number of available characterisation factors for chemicals and their quality. This will primarily improve the comparability of LCA-ecotoxicity results between products. Option three builds on this and aims at harmonising the use of ecotoxicity data between LCA and ecological risk assessment. It consists of changing the ecotoxicity reference data from the geometric mean of the EC_{50}-values (current in USEtox) to the PNEC (Predicted no effect concentration), which protect the most sensitive species. The last option is not to change the assessment and to obtain an understanding of the discriminative power of the current ecotoxicity assessment in USEtox.

1. INTRODUCTION

1.1 Remit of the Task Force and Purpose of this Report

There is increasing interest from regulators to apply life cycle based impact assessment methodologies to assess in a comparative way the environmental performance of chemicals as well as products, and to include freshwater ecotoxicity as an impact category. Examples include initiatives on green chemistry and The Sustainability Consortium (TSC) in the USA, the Grenelle Regulation in France and, especially, the EU's Single Market for Green Products Initiative that covers both fast moving consumer goods as well as durable goods. This initiative encompasses the Product Environmental Footprint (PEF) pilot project, which includes some 25 test categories from the food and non-food sector (http://ec.europa.eu/environment/eussd/smgp/policy_footprint.htm).

The objective of such initiatives is the broad assessment of the environmental impact of products with multiple indicators. Of specific interest to this ECETOC Task Force is the application of the USEtox method (Rosenbaum et al, 2008) for measuring freshwater ecotoxicological impacts. Whereas some models are generally accepted now, others are still under discussion. The USEtox method is typically in the latter situation even though UNEP and SETAC have declared it as their consensus model. The European PEF project is the first large-scale application of USEtox to a variety of in-market products. The results of the pilot project on 'household detergents' implies that aquatic ecotoxicity as assessed by USEtox is a major impact category (AISE, 2015). At the same time, the results of individual chemical prospective risk assessments and of retrospective eco-epidemiological observations do not give evidence of actual impacts. Hence, it appears timely to investigate the readiness and suitability of this method in view of its intended use for comparing the environmental profile of consumer products based on aquatic (freshwater) ecotoxicity impact.

To this end, the extension of the traditional LCA methodology to include the ecotoxicological impacts of chemicals, products and/or services is addressed vis-a-vis the accepted norm within the industry and the regulatory world, which is to use risk assessment to manage chemicals in society.

At the same time, the Scientific Committees of the EU have outlined that current prospective environmental risk assessment methodology is far from being realistic, i.e. delivering an accurate approximation of the environmental impact of chemicals (SCENHIR, SCCS, SCHER, 2012). However, there has been no detailed assessment either of whether decisions based on an LCA-based ranking (such as USEtox and CDV), result in a better and more realistic control of environmental impacts. Real practical assessment and decision-making problems arise for the industry in situations where different ecotoxicity assessment methods point to different causes and solutions. This may stall progress in the area of chemical management.

With this in mind, this ECETOC Task Force was chartered to:

1. Conduct a scientific evaluation of the USEtox method, currently the leading method for calculating toxicity impacts in LCA, and its relevance to the real world;
2. Investigate the relationship of USEtox to chemical risk assessment methodology;
3. Provide guidance on the scientific relevance and interpretation of USEtox results in the context of chemical impact assessment and selection of chemical-based (manufactured) products.

Three 'work streams' were identified that have been guiding the task force work and organisation:

Comparison and in-depth analysis of tools

- Scientific evaluation of the USEtox method and its relevance to the real world;
- Comparison of USEtox to other ecotox impact methods such as CDV;
- Provide guidance on the scientific relevance and interpretation of USEtox results regarding selection and/or ranking of chemical-based products.

Study the influence of LCA best practices on the USEtox ecotoxicity results

- Practice of modelling with LCA databases and influence on the ecotoxicity results;
- Data availability and treatment of missing data.

Comparison of the purpose and scope of LCA and Risk Assessment

- Comparison of LCA and Risk Assessment fundamentals;
- Potential for reusing methods of risk assessment in LCA;
- Guidance on how both kinds of assessment can be used in conjunction with or complementing each other.

The purpose of this report is, therefore, to discuss in a condensed way the interface between different available methods to assess and manage ecotoxicity of chemicals and chemical-containing products in the industry. To that end, ecological risk assessment and the ecotoxicity assessment in life cycle assessment will be compared to each other (Chapter 2). The 'Critical Dilution Volume' method and additional ecotoxicity assessment approaches are presented in Chapter 3. A simple 'virtual' product was assessed according to the LCA and the CDV methodology (Chapters 4 and 5). This served to exemplify several of the discussion points. Chapter 6 discusses the degree of certainty of the results with regard to approximating the ecological impact. Chapter 7 provides suggestions for a way forward, taking into account the outcome of the previous chapters. These suggestions are intended to be the starting point of multi-stakeholder discussion. This report will be based on prominent examples of the current European discussion, i.e. the methodology used in the European legislation on industrial chemicals (i.e. REACH) and a methodology which is used in a European project which pilots the holistic assessment and comparison of product (i.e. the Product Environmental Footprint (PEF) project). The authors have attempted to avoid the excessive use of LCA and ERA 'jargon', but expect the reader to have a basic familiarity with the principles and data needs of both assessment methodologies.

1.2 Introduction to ERA and LCA in the Context of Chemical and Product Evaluations

Risk assessment (RA) and life cycle assessment (LCA) are two analytical tools used to support decision making in environmental management. RA and LCA were initially developed and used by largely separate communities of specialists. In the context of environmental management, RA is often concerned with evaluating the risks posed by stressors, such as chemical pollutants or pathogens, to humans and other receptors. Risk is commonly defined as a combination of the probability of occurrence, and the severity

(nature and magnitude) of adverse effects from a proposed action. The quantitative assessment of chemical risks to the environment is often labelled as ecological risk assessment or environmental risk assessment (ERA) (Harder et al, 2015).

ERA: Environmental Risk assessment evaluates the likelihood of harmful consequences as result of a condition or action on the environment, caused by human activities. The objective is the evaluation of the need for risk management to avoid or limit the impact of chemicals on the environment. Many activities result in the emissions of chemical substances into the environment with subsequent consequences. ERA involves assessing both the hazards and exposure following the release of chemicals in hypothetical or real future scenarios, for risk management (van Leeuwen and Vermeire, 2007). "ERA is a process that incorporates technical information and societal values in arriving at risk management options" (UNEP, 1999). In view of the objective and due to the potential complexity of the assessment, ERA can be implemented as a tiered process, starting with a screening process and a reduced set of input parameters, followed by subsequent refinement when necessary. At the screening stage, the need for deeper evaluation and eventual risk management is ruled out for low-risk cases, while the higher risk cases are evaluated at an increasing level of detail. From that perspective, ERA needs to be conservative at the onset: one of the prerequisites is starting with conservative assumptions that will lead to an attribution of maximum risk in the absence of information and a potential reduction of risk as more knowledge is gathered on both chemical hazards and exposure. However, in order to arrive at effective risk management options, the degree of conservatism needs to be reduced such that at a sufficient level of refinement a realistic evaluation of the possible impact of a chemical is obtained.

Performing ERA is a requirement under the EU REACH regulation for industrial chemicals (EC, 2007), and similar risk-based regulations exist in other geographies. The goal of ERA in a regulatory context is not only to show whether there is a risk or not but also to describe the conditions under which the risk can be controlled and/or reduced to avoid the occurrence of adverse effects. Besides, the EU requires ERAs in the course of admitting plant protection products (EC, 2008), biocidal products (EU, 2012), veterinary medicines (EC, 2001a) and human medicines (EC, 2001b) to the EU markets.

LCA: LCA is an analytical tool for the (comparative) environmental assessment of products or services and generally covers the entire life cycle, or supply chain, of a product or service. Environmentally relevant resource consumption and emissions throughout this life cycle are quantified with respect to an arbitrarily chosen 'functional unit' (FU), and the related potential impacts on a number of safeguard subjects (e.g. human health, natural environment, and natural resources) are estimated. The environmental 'safeguard subjects' covered by LCA at 'endpoint level' are typically defined more holistically than the test species or ecosystems protected in ERA.

LCA methodology has developed considerably since its emergence in the late 1970s, and several life-cycle inventory (LCI) databases and life-cycle impact assessment (LCIA) methods are available today. LCIA methods cover a continuously expanding number of impact categories and corresponding characterisation models for the conversion of emissions from, and resources used in the life cycle of a product or service, into impacts. This type of LCA may also be referred to as environmental LCA (E-LCA) in order to distinguish it from social LCA (S-LCA) and life cycle costing (LCC). Both RA and LCA can be used to evaluate the effects of chemical pollutants and pathogens emitted to the environment on humans and other species. Both tools require quite similar

information about emissions, fate, and transport in the environment, exposure, and effects on different receptors (Harder et al, 2015).

Early attempts to include human toxicity and ecotoxicity of chemical pollutants in LCA were to a large extent inspired by expert knowledge and mathematical relationships established within chemical RA. In a similar way, early efforts to include the effects of pathogens on human health in LCA were largely inspired by the quantitative assessment of pathogen risks, usually labelled as quantitative microbial risk assessment (QMRA). The similarities, differences and potential synergies between RA and LCA have been thoroughly discussed and reviewed by Harder et al (2015), and references cited therein.

1.3   Current Regulatory Context for Industry

The possibility for industry to use and market chemicals in Europe (as individual substances or as part of products and articles) is regulated by the REACH Regulation (EC) No 1907/2006 (EC, 2007) . REACH is a regulation of the European Union, adopted to improve the protection of human health and the environment from the risks that can be posed by chemicals while enhancing the competitiveness of the EU chemicals industry. In principle, REACH applies to all chemical substances; not only those used in industrial processes but also in our day-to-day lives, for example in cleaning products and paints, as well as in articles such as clothes, furniture, and electrical appliances. Therefore, the regulation has an impact on most companies across the EU. If the risks cannot be managed, authorities can restrict the use of substances of concern in different ways. In the long run, the most hazardous substances should be substituted with less dangerous ones [http://echa.europa.eu/regulations/reach/understanding-reach].

In 2008, the European Commission (EC) also published its *Action Plan on Sustainable Consumption and Production* (SCP/SIP), including various proposals for a number of tools such as Ecolabel, Energy Label, Ecodesign, Retail Forum, and others. The launch by the EC of the Resource Efficiency Roadmap followed in September 2011; the communication on 'Building the Single Market for Green Products (SMGP) – Facilitating better information on the environmental performance of products and organisations' was released on 9 April 2013. The recent publication of the Resource Efficiency Roadmap (http://ec.europa.eu/environment/resource_efficiency/index_en.htm) has further strengthened and defined the future role of the environmental footprint methodology by explaining that the Commission will:

- Establish a common methodological approach to enable the Member States and the private sector to assess, display and benchmark the environmental performance of products, services and companies based on a comprehensive assessment of environmental impacts over the life cycle ('environmental footprint') (in 2012);
- Ensure better understanding of consumer behaviour and provide better information on the environmental footprints of products, including preventing the use of misleading claims, and refining eco-labelling schemes (in 2012).

The EC (2010), working closely with the Joint Research Centre (JRC), has developed two methods to measure the environmental performance throughout the life cycle, the Product Environmental Footprint (PEF) and the Organisation Environmental Footprint (OEF) (http://ec.europa.eu/environment/eussd/smgp/policy_footprint.htm). The methodologies are based on

the LCA technique and the International Reference Life Cycle Data System ILCD handbook (2010) as well as other existing standards and guidance documents, including ISO 14040/44, ISO/TS 14067, ISO 14020, PAS 2050, BP X30-323, WRI/WBCSD GHG Protocol.

The aim of PEF is to develop a harmonised methodology for the calculation of the environmental footprint of products. A reliable, credible and consistent measure of this environmental footprint is a fundamental step in raising business and consumer awareness of potential impacts, thereby helping to reduce that footprint. In order to achieve this, rules have to be developed for individual product categories to allow consideration of specific product-level details.

In this regard, some 25 pilot projects are currently running from 2013 – 2016 that will develop so-called Product Environmental Footprint Category Rules (PEFCRs) per industrial sector (EC, 2013a). Current efforts regarding the EU PEF initiative suggest that likely additional legislation or demands on industry will surface based on LCA, leading to Business-to-Business (B2B) and or Business-to-Consumer (B2C) environmental information influencing the marketability of products.

Environmental RA and LCA have a different conceptual basis but do share common categories of analysed impacts, which turn out to create potential problems and contradictions in a market context that will be discussed further in this document.

2. ASSESSING ECOTOXICITY IMPACT - COMPARISON OF RA AND LCA

2.1 Introduction – Regulatory Status of the Assessments and available guidance

RA is a regulatory prerequisite to be compliant with chemical regulations in the EU, such as plant protection regulation, the biocidal products directive and REACH for industrial chemicals. The obligation to conduct an RA for single substances to gain access to the chemical market is a fundamental principal in European chemical regulations. Only substances that are safe in the scope of RA can access the markets (EC, 2007).

There is a general demand, particularly for industry, to put their risk assessment for individual chemicals into a more holistic context. On the one hand, that means to assess environmental impacts along the entire value chain. In addition, there is the demand to widen the scope of the assessment by including impacts other than ecotoxicity such as eutrophication, climate change etc. LCA is a methodology which allows for this.

So far, LCA is largely used on a voluntary basis. However, the French Grenelle regulation requires participating companies to assess the climate change impact of goods by LCA. As part of the EU's Single Market for Green Products Initiative, the European Union has launched two pilot projects to test LCA methodology for assessing the organisation of environmental footprint (OEF) and product environmental footprint (PEF). The latter covers both fast moving consumer goods and durable goods. The ultimate intention of the PEF is to develop a metric base on which products can be compared with regard to their environmental impact (Askham, 2012; EC, 2007).

LCA on the other hand currently does not have a legally binding function but is a valuable method to compare different products and/or services and determine possible impacts on the environment along the entire value chain including the raw materials (Askham, 2012). Its use is generally considered as complementary to ERA.

The goal of LCA is to identify the most efficient ways to reduce the impact on human health and environment of these substances authorised on the market. The PEF project under development intends to fix the LCA methodology for specific product categories in a way that would allow a reliable comparison between consumer products from the same 'category', such as shampoos or detergents. Consequently, the PEF Guide (EC, 2013a) is more precise than ISO 14040:2006 guideline, via the use of so-called 'category rules'. Also, specific models have been agreed to evaluate impacts for each impact category.

The aquatic ecotoxicity assessments in LCA and RA deal with similar topics and use similar data. Both methods have much in common, but follow different strategies to achieve different assessment goals. The similarities and the differences among the two methods are presented in this chapter. Additionally, the specific tools used in risk assessment (EUSES-based tools) and in LCIA (USEtox for ecotoxicity impacts) are highlighted to further illustrate the similarities and the differences. Where possible, guidance is given on how both kinds of assessment can be used in conjunction with or complementing each other.

2.2   Objectives and Scopes

Both methodologies fulfil different purposes and can therefore not replace each other. Looking at ecotoxicity, they both can be used to guide the reduction of chemical impact on the environment. Specifically, risk assessment (RA) is performed to find out whether the use of an individual chemical can be considered safe, i.e. not resulting in a deleterious impact on the environment. Typically, RA can be carried out in a tiered approach, which may start data-poor and in which missing data are compensated for with worst-case assumptions. If required, RA can be refined, e.g. by adding data or by replacing lower-tier with higher-tier input information.

Due to the nature of the question, the numerical result of the assessment is of limited relevance because the specificity of the input information can be increased, which has a direct impact on the outcome. Vice-versa, the uncertainty of the input information and the degree of conservatism is reduced by using higher tier data. In such an iterative process, the assessment can be refined with information until a final conclusion can be reached. Please note that the refinement of the input information is both time- and cost-intensive.

The objective of the aquatic ecotoxicity assessment in LCA is different. It is to quantify the impact related to the emissions of all chemicals along the entire life-cycle of a product or service. The overall result is obtained as the sum of the result for all chemicals.

2.3   Ecotoxicological Risk Assessment - Principles

The standard approach of RA includes four different phases, which are summarised below (EU TGD Part II, 2003; van Leeuwen and Vermeire, 2007).

1. Hazard identification;
2. Dose (concentration) – response (effect) assessment;
3. Exposure assessment;
4. Risk characterisation.

2.3.1   Hazard identification

In the first step, the effects of concern are identified and the hazard classification of the substance according to GHS (Global Harmonised System) is established or reviewed.

2.3.2   Dose – response assessment

In the dose (concentration) – response (effect) assessment, the predicted no-effect concentration (PNEC) is developed. For both steps, it is of high importance to evaluate the data with regard to their adequacy, relevance, and completeness. For the derivation of the PNECs, all available data should be taken into account. The adequacy of data is generally evaluated with a scoring system according to Klimisch et al (1997). This system has four scores (1: reliable without restrictions; 2: reliable with restrictions; 3: not reliable; 4: not

assignable) and is used throughout the registration works for REACH. In principle, only data from categories 1 and 2 should be preferred. Data from category 4 might be used in a weight-of-evidence approach. From several studies a key study needs to be chosen which is then used for the derivation of the PNEC (Predicted No Effect Concentration) by applying appropriate assessment factors to account for the extrapolation from acute to chronic exposure, for the variability between experimental data, and for the uncertainty in extrapolating from single species data to a population. The PNEC is the threshold concentration which must not be exceeded in order to avoid deleterious effects on the environment.

2.3.3 Exposure assessment

In the subsequent exposure assessment, the environmental concentrations are determined either by using/gathering environmental monitoring data, or more commonly by modelling exposure in a hypothetical standard environment.

The starting point of the exposure assessment in predictive modelling is to define the use of a chemical and the rate Q at which the chemical is used (e.g. kg/day or tons/day). In order to define the emissions to the environment, release factors to water, air and soil are defined (Reihlen et al, 2016). A variety of sources is available to that end. (Reihlen et al, 2016). The emissions E to water, air, and soil are obtained according to equation (1).

$$E_{Air\,/\,Water\,/\,Soil} = Q * RF_{Air\,/\,Water\,/\,Soil} \qquad (1)$$

The emissions are an input to multimedia fate modelling. For REACH the EUSES model is employed (ECHA, 2016). It represents the environment as a nested set of boxes which are in exchange with each other (Brandes et al, 1996). It accounts for partitioning between compartments, degradation reactions and advective transport between compartments / boxes. The multimedia fate model yields so-called predicted environmental concentrations (PECs).

To ensure realistic PECs, all relevant exposure-related information on the substance is used. The PECs are derived for every single use of the compound and for every environmental compartment. Due to the lack of monitoring data, modelled PECs are usually used and the user has the option to refine his underlying modelling assumptions from conservative default parameters to more realistic conditions.

2.3.4 Risk characterisation

Calculation of RCR

The last step encompasses the risk characterisation in which the PEC and PNEC values for the different environmental compartments are used to develop a risk characterisation ratio (RCR = PEC/PNEC for a given compartment) which needs to be below 1.0. If this is not the case, further refinements must be done to ensure an RCR < 1, e.g. the use of risk management measures (RMMs) or the generation of additional experimental toxicity data to reduce the assessment factor.

Tiered approach

As described for instance by van Leeuwen and Vermeire (2007), risk assessment is often a tiered approach. This is possible since the goal of the risk assessment is to assess whether PEC is below PNEC. In order to be resource efficient, the assessment often starts with conservative assumptions. If necessary, these conservative assumptions are replaced with less conservative assumptions, and if needed and possible with measured data. In this manner, the realism of the assessment is increased. There are multiple refinement options. For exposure modelling, these include replacing very generic emission estimation by measured release rates, replacing partition coefficients derived from quantitative structure-activity relationships with measured partition coefficients, using geo-referenced models (GREATER) rather than EUSES. Another option is to use measured environmental concentrations rather than predicted values. Finally, the effect threshold can be refined by using chronic instead of acute ecotoxicity data. Even further refinement is possible, e.g. the use of mesosome data or by species sensitivity distributions (SSDs).

For the sake of transparency, it is crucial that every deviation from default parameters needs to be documented and justified. At the end of the process, the entire assessment has to be communicated both to the authorities and to the downstream users handling the substance. The downstream users are then obliged to verify that they handle the compound in a way which is in compliance with the boundaries described in the assessment.

2.4 Life Cycle Assessment – Principles

Life Cycle Assessment (LCA) predicts the impact of a product / service in a cumulative manner overall life cycle stages or a defined subset of life cycles stages of a product. Identification of 'hotspots' in the life cycle is often the first objective when dealing with a product / service not yet analysed, but a quantitative comparison is also possible and often attempted. Both identified 'hotspots' and quantitative comparisons can subsequently influence decision making. In the scope of PEF, a quantitative comparison is pursued. Products are benchmarked against a defined category standard with the aim of providing consumers with information to make an informed decision when purchasing a product as to which product shows a comparatively better environmental performance.

The approach to LCA has been formalised in ISO norms 14040/44, which divide the process into four phases (ISO 14040:1997, ISO 14044:2006):

1.   Goal and Scope of the assessment
2.   Life cycle inventory (LCI)
3.   Life cycle impact assessment (LCIA)
4.   Interpretation of the results.

2.4.1 Goals and Scope of the assessment

Defining the goal and scope of the assessment is the first logical step to determine the boundaries of the assessment (e.g. cradle-to-gate or cradle-to-grave). At this step, it should also be clear which impact categories are to be analysed in the scope of the study for a focused data collection in the subsequent steps in the LCA.

2.4.2 Life Cycle Inventory

During the subsequent life cycle inventory (LCI) analysis, the material flows that are relevant to the specific product need to be described. In principle, this inventory can be characterised as a vector of flows (Heijungs and Suh, 2002). Material flows which characterise products and intermediates are termed 'intermediate flows' and occur within the 'technosphere', i.e. that part of the world which covers the production and use of products. Flows from and to the environment – also termed the 'biosphere' in LCA – are named 'primary' flows or 'environmental interventions'. These primary flows are those that are evaluated in the impact assessment, whereas intermediate flows here only serve to scale the primary flows to the correct proportions and will not be scored. Primary flows are directed towards specified environmental compartments, but the precise definition and number of compartments depends on the database provider. Any production chain captured by these database models can be very complex and can be represented as tree structures, such as the one depicted in Figure 2.1. Each string in the illustration symbolises an LCI of its own. All these LCIs are linked towards the level 0 dataset of the depicted tree and can have their own emissions (primary flows) that will be evaluated in the LCIA step.
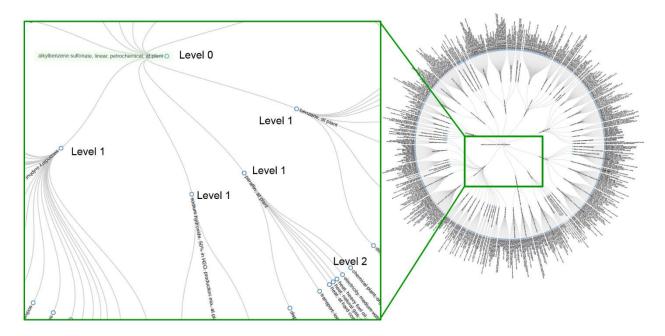
Figure 2.1: Illustration of several levels of the life cycle inventory analysis and its possible flows

In Figure 2.1, the string at level 0 stands for a dataset selectable in an LCA database, here 'linear alkyl benzene'. Implicitly the database links to further datasets, represented by level 1, to fulfil the functional unit defined at level 0. The datasets at level 1 link to further datasets and so on and so forth. The user of the database is usually not confronted with this complexity, as the providers of databases offer aggregated datasets that provide the results of the linking operation in one compact dataset. While being compact, this format does not allow the user to analyse in detail from where emissions in specific models stem.

Information on flows is compiled in publicly available databases. These may differ in the precise definition and number of compartments. In view of the complexity of material flows in an entire life cycle, collection of this data is practically not feasible. Hence, the LCA practitioner has to rely on publicly available databases such as Ecoinvent (Frischknecht et al, 2005), GaBi[1] or ELCD[2] to fill data gaps and to cover data outside of the practitioner's direct grasp. For example, the LCA practitioner may know the size of emissions during the production stages occurring in their own production site as well as the consumption of electricity. While the emissions in their own production are then directly available and can be entered in the LCI, the emissions due to the consumptions of electricity would still be unknown. The practitioner would then typically specify the known energy demand in a software frontend and insert a link to a ready-made model for electricity from one of the above-mentioned databases. These readymade models typically cover all prior steps leading to the final equivalent of energy required to fulfil the functional unit. The importing of all emissions associated with the production of electricity is automatically done by the software.

Emissions of the same type (e.g. CO_2 to continental air) will be summed up in an aggregate figure for the entire dataset. In the case study, the use of a product consisting of several chemicals is assessed and hence all emissions related to these chemicals. This includes the emissions resulting from the production processes, the generation of electricity used in the substances life-cycle, and the down-the-drain disposal. Thus the ecotoxicity assessment addresses a suite of chemicals that is much wider than those contained in the product.

2.4.3   Life Cycle Impact Assessment

Impact calculation

The subsequent impact assessment deals with the significance of potential impacts. Therefore, impact scores need to be derived for the relevant impact categories. In the practice of LCA the calculation of the impact follows a straightforward calculation (Heijungs and Suh, 2002) that can be described by the formula

$$Impact = \sum_i LCI_i \cdot CF_i \ .$$
(2)

---

[1] EC, 2013a. The overall methodological framework1 GaBi database, http://www.gabi-software.com/international/databases/ is given by the PEF Guidance (EC, 2013b)

[2] European reference Life Cycle Database, http://eplca.jrc.ec.europa.eu/ELCD3/index.xhtml

In this sum, we assume each element LCI_i to be a primary flow or environmental intervention (emission flows into specific compartments in the environments in the case of environmental ecotoxicity). For each such primary flow a corresponding characterisation factor CF_i is defined (possibly also undefined, see discussion below). The calculation of each CF within this vector can be the result of more complicated calculations and we describe the procedure used for the assessment of ecotoxicity using USEtox in chapter 3 below. The actual calculation of the impact score then follows, however, the routine is simple and described by the preceding formula.

This corresponds to the following representation in vector notation:

$$\boldsymbol{Impact = \overrightarrow{LCI} \cdot \overrightarrow{CF}} \qquad\qquad (3)$$
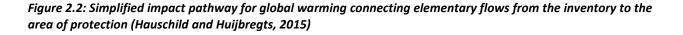
As described in the previous section, all elementary flows of the same type are summed up in the same position of the $\overrightarrow{LCI}$ vector. The step of substitution is something usually completed by the providers of LCA databases and not performed by the user. The LCA practitioner only selects an appropriate dataset and for a service, process or product and $\overrightarrow{LCI}$ is then made available automatically. The number of elementary flows used in a database by default can be very large and is typically on the order of thousands of flows. Most datasets have small, but non-zero contributions in all positions of the emission vector due to the fact that in LCA all upstream elements are considered (please refer to Figure 2.1). $\overrightarrow{CF}$ is the vector of characterisation factors and has the same dimensionality as $\overrightarrow{LCI}$.
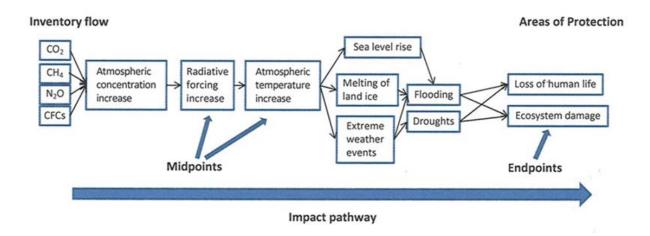
While the model behind the calculation of CFs can be of arbitrary complexity, the LCIA as described by equations (2) and (3) has implicit limitations. Each element of $\overrightarrow{CF}$ has exactly one corresponding element in $\overrightarrow{LCI}$ and the sum of all pairwise products make up the impact. As a result, the impact is the sum of all individual contributions. Considering correlations between single contributions is not possible in this model. This is also the current status in the assessment of mixtures (ECETOC, 2011).

To perform an LCA, impact models are needed. These models can be seen as toolboxes where *Characterisation Factors* (CF) linked to different impact categories are gathered by impact category. In each impact category (*e.g.* climate change, resource depletion - water, freshwater ecotoxicity), all flows collected during the *Inventory phase* are multiplied by the appropriate CF to turn them into results expressed with the same specific quantitative unit. These results can thus be aggregated by impact category.

Endpoint and Midpoint Models
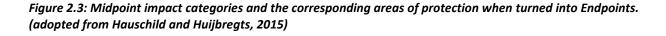
Depending on the specificities of the CF, different types of models are distinguished referring to different 'locations' on the impact pathway linking inventory data through consecutive environmental impacts to damage that they cause on different areas of protection (Hauschild and Huijbregts, 2015). Figure 2.2 illustrates the difference between Midpoints and Endpoints when considering the impact pathway for global warming.

Figure 2.2: Simplified impact pathway for global warming connecting elementary flows from the inventory to the area of protection (Hauschild and Huijbregts, 2015)
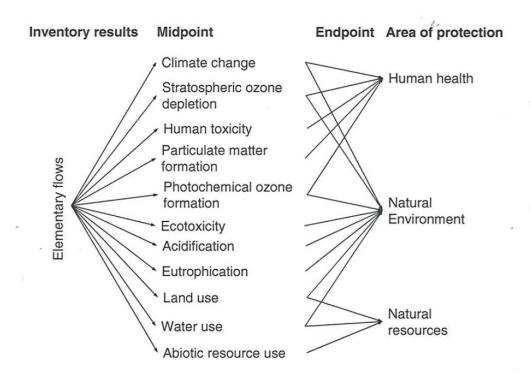
These two steps in the impact pathway lead to two types of impact models:

- Midpoint models: these models reflect *Impacts* induced by each Life Cycle phase on the environment. CFs convert extractions and emissions into midpoint results expressed in the quantitative unit of their corresponding impact category, such as m^3 of water, kg CO_2 equivalent, CTUe (Comparative Toxic Unit equivalent), etc. Midpoint results of a given impact category expressed with the same quantitative unit, can then be aggregated by Life Cycle phase or even on the whole Life Cycle of a product.

- Endpoint models: *Impacts (i.e.* midpoint results per impact category*)* can be transformed into *Damage (i.e.* endpoint results), in order to estimate the effects on 'safeguard subjects' as illustrated in Figure 2.3. For instance, Endpoint results estimate effects on Human health or on Ecosystem quality and can be respectively expressed in DALY (Disability Adjusted Life Year) or in $PDF.m^2.y$ (Potentially Disappeared Fraction of species on 1 m^2 during one year because of pressure induced on the considered ecosystem).

Figure 2.3: Midpoint impact categories and the corresponding areas of protection when turned into Endpoints. (adopted from Hauschild and Huijbregts, 2015)

Whatever the impact category considered, different models (endpoint and midpoint) exist. Indeed, since LCA appeared, models have been enriched and new methodologies have been proposed resulting consequently in various methods. As a result, there is a call for further harmonisation and streamlining of LCIA, with the USEtox project and the ILCD Handbook (JRC-IES, 2011) being examples of such efforts.

Aquatic ecotoxicity assessment methods

The Joint Research Centre and Integrated Environmental Solutions published in 2011 the ILCD (International reference Life Cycle Data system) Handbook (JRC-IES, 2011). This Guide analyses the impact assessment methods to select the most appropriate ones in the European context.

The different methods to assess impacts related to Ecotoxicity are presented in Table 2.1.

Table 2.1: Selected midpoint methods and underlying models for ecotoxicity (adopted from JRC-IES, 2011)

Midpoint method	Underlying model	Reference
USEtox	Model developed under auspices of UNEP/SETAC Life Cycle Initiative	Rosenbaum et al, 2008
ReCiPe[a]	USES-LCA version 2.0	Huijbregts et al, 2009
IMPACT 2002+[b]	IMPACT 2002	Jolliet et al, 2003
TRACI	CalTOX 4.0	Bare et al, 2003
EDIP2003[c]	EDIP1997, combined with site-dependent factors	Tørsløv et al, 2005
Swiss Ecoscarcity	Based on a combination of actual emissions and emission limit values	Frischknecht et al, 2008
MEEuP	Based on emission limit values	Kemna et al, 2005
Endpoint Method		
EPS2000	Based on a combination of red list species supposed to be threatened by chemicals and total emission loads	Steen, 1999a, b
ReCiPe[a]	USES-LCA version 2.0	Huijbregts et al, 2009
IMPACT 2002+[b]	IMPACT 2002	Jolliet et al, 2003

[a] The most recent version of the model USES-LCA is the underlying model for the calculation of characterisation factors for ecotoxicity in ReCiPe. Previous versions of the model family USES-LCA and EUSES, employed in CML2002 and Eco-indicator99, were not included in the evaluation.

[b] The European version of the model IMPACT2002 is the underlying model for the calculations of characterisation factors for ecotoxicity in IMPACT2002+. LUCAS and LIME contain respectively Canadian and Japanese versions of IMPACT2002 and were not included in the evaluation.

[c] The most recent version of the EDIP method is evaluated (2003 version). A previous version, EDIP1997, was not included in the evaluation.

The emissions defined in the Life Cycle Inventory (see 2.4.2) are the starting point for the ecotoxicity assessment. These emissions can occur into different compartments of the environment (e.g. air, soil, freshwater, marine water).

According to their fate modelling, these methods can be divided into three groups:

1. Full multimedia fate modelling (USEtox, ReCiPe, IMPACT2002+, Caltox (TRACI);
2. Partial fate modelling - Environmental key properties (EDIP);
3. No fate modelling (Swiss Ecoscarcity and MEEuP).

Multimedia fate models have been developed to calculate the concentrations resulting from these emissions in freshwater, terrestrial or marine ecosystems. Depending on the physico-chemical properties of the substances emitted and of the compartment of emission, the potentially ecotoxic substances either remain in the compartment of emission or move to another compartment (see Figure 2.4). Some are quickly degraded. Others can persist in the environment. Ecotoxicity on species thus may vary with the Fate of emitted substances.

The ILCD guide finally comes to the point that: "*USEtox is preferred as the recommended default method for the midpoint evaluation of freshwater ecotoxicity impacts. […] It results from a consensus building effort amongst related modellers and, hence, the underlying principles reflect common and agreed recommendations from these experts. The model accounts for all important parameters in the impact pathway as identified by a systematic model comparison within the consensus process. The model addresses the freshwater part of the environment problem and includes the vital model elements in a scientifically up-to-date way.*" (JRC-IES, 2011).

Eventually, USEtox was selected to evaluate ecotoxicity impacts on Freshwater compartment in the European PEF project. In this project, USEtox is even the sole one recommended today for impact assessment of chemicals on the aquatic environment.

Reliability and Accuracy in LCIA

An important factor in the reliability of the assessment of ecotoxicity (as well as other impact indicators) is the completeness of data used in the LCA. As described in section 2.4.2 emission flows of the foreground system, i.e. those life cycle steps in the focus of the assessor, would be added manually, while flows of the background system (e.g. electricity) will be filled in automatically by the software system and database used.

The following situations are typical in the calculation of the LCIA:

1) CF_i is not available for an emission flow LCI_i (equivalent to an element of $\overrightarrow{CF}$ being undefined);
2) CF_i is uncertain;
3) LCI_i is uncertain, inaccurate.

The situations described in the preceding list can have an influence on the overall uncertainty of an LCA impact score.

Situation 1) leads to the impact for an emission flow to be calculated as zero, thus making no contribution in the overall score. This can be sensible if the element LCI_i for which CF_i is undefined is assumed not to make an impact in the selected impact category (e.g. 'emission of sodium chloride to river water' on global warming). But it would constitute a factor of uncertainty in the general sense, as it may not be easy to see for non-experts in an impact category whether this assumption is justified.

Situation 2) can be due to the model used to calculate the characterisation factors having uncertainties as well as the data fed into to model being inaccurate.

Situation 3) can have apparent differences of datasets as a reason or be due to the use of old or uncertain (e.g. estimated) data. With apparent differences, we mean the differences that result when two independent LCA practitioners are tasked with the creation of a common dataset. Since LCI datasets are complex objects, there are opportunities for both assessors to take different choices in many places in their modelling approach. Also, they may apply entirely different levels of scrutiny in assembling the LCI, resulting in a datasets of varying level of detail. Since in LCA a 'best case' approach is adopted, an item that is not present in the LCI will have zero impact, disfavouring the most detailed model. As a result of the work of the two practitioners two different vectors $\overrightarrow{LCI}$ may be fed into the LCIA resulting in seeming differences for the same process.

While in principle it would be possible to address all described issues in a single LCA, the sheer number and high degree of interlinkage of data in the $\overrightarrow{LCI}$ and $\overrightarrow{CF}$ make this a challenge, thus effectively rendering the calculation result intransparent for all normal users of an LCA. According to experience and communication with other expert LCA practitioners, these issues affect the experts as well.

Issues 1) and 2) could be made transparent by defining an automated assessment of data quality including a binding standard how to assign data quality levels to datasets, eventually penalising data gaps and poor data. By default, all characterisation factors for primary flows that are not relevant in an impact category could be set to zero. Issue 3) is much more difficult to address, since a common standard is difficult to define at the level detail that would be required to ensure a comparability of datasets. The existing common guidelines for LCA are not currently helpful.

So, uncertainty assessment in LCA and for the ecotoxicity impact assessment methods, in particular, is complex and multifaceted. Uncertainty insights are critical to be able to determine what minimal differences between alternatives need to be observed before a difference can be deemed statistically significant. This can be studied at the level of the calculated CF, but in the context of this report the uncertainty at the level of a calculated ecotoxicity score for a full product is the key question.

For the ecotoxicological effect factor, as used e.g. in the USEtox method, good insights are provided in the paper by van Zelm et al (2007). Depending on the mode of action, and the number and type of species tested, the uncertainty on the effect factor is at least two orders of magnitude. This needs to be further combined with the uncertainty on the fate and effect factors. As a result, the expected uncertainty on ecotoxicity characterisation factors is very substantial. This is further complicated by the mixing of different data types (e.g. QSAR versus experimental data) and data sources. While a quantitative assessment of uncertainty around the ecotoxicity scores of different product options needs further elaboration, it is very likely that it spans several orders of magnitude. By contrast, many consumer products are formulated in very similar ways, and calculated (small) differences in ecotoxicity score may be statistically irrelevant.

2.4.4 Interpretation of the results

The results from the above-mentioned phases described in § 2.4.1 to 2.4.3 are then discussed in the final interpretation to conclude on the overall environmental footprint.

Impacts all along the life cycle are grouped together and added. This allows a comparison of the global impact of the functional unit studied with an alternative scenario or another product studied using the same functional unit. LCA can thus be applied to evaluate environmental improvements linked to a (new) product.

Furthermore, impacts of each step of the life cycle are determined. Identifying the most impacting steps (so-called hotspots) can help reducing impacts more efficiently.

For a good understanding of the underlying approach and merits of ERA and LCA methodologies, an important conceptual difference should be pointed out: in deriving the ecotoxicity element of the assessment, ERA methodology assumes that there exists a threshold concentration value below which a chemical is not harmful anymore (the NOEC [No observed effect concentration] for individual species, and the PNEC for the

ecosystem), whereas LCA assumes a continuous relationship between concentration/dose and ecotoxicity. This fundamental paradigm difference is at the basis of the different application of both methodologies.

2.5 RA and LCA comparison

RA and LCA are two approaches used to respectively assess risks and impacts on the environment. For both approaches, several models were developed. Under the REACH context and the PEF project, two models are recommended: EUSES for ERA and USEtox for LCA. Figure 2.4 sums up RA and LCA approaches.
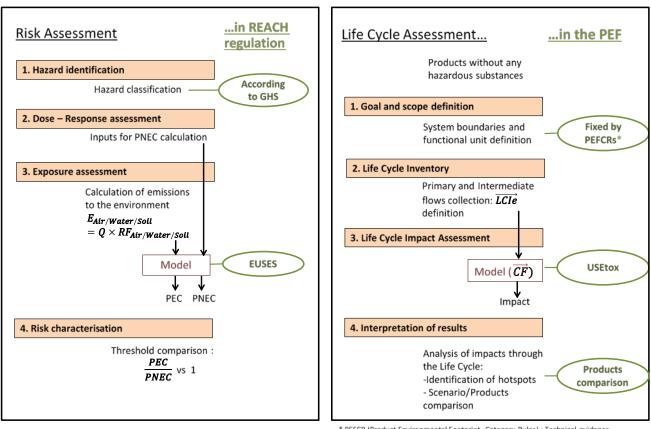
Figure 2.4: RA and LCA principles for assessing Freshwater ecotoxicity under the current regulatory context

The following paragraphs aim at comparing RA and LCA methodologies principles.

2.5.1 RA and LCA: Commonalities

Compartments of concern in RA and LCA

Historically, freshwater was the only relevant compartment in RA and ecotoxicology in general which is reasonable considering that compounds usually enter the environment *via* releases from sewage treatment

plants and end up in surface waters. However, in today's methodology RA must evaluate multiple environmental compartments because, due to their intrinsic physical-chemical properties, chemicals will distribute differently in the environment and water might not always be the compartment of concern. The compartments RA has usually to deal with are listed below (EU TGD Part II, 2003; van Leeuwen and Vermeire, 2007).

- For inland risk assessment
    o Aquatic ecosystem (including sediment)
    o Terrestrial ecosystem
    o Top predators *via* the food chain (secondary poisoning)
    o Microorganisms in sewage treatment systems
    o Atmosphere
- For marine risk assessment
    o Aquatic ecosystem (including sediment)
    o Top predators via the food chain (secondary poisoning)
- Man via the environment

Principally LCA can deal with any number/type of environmental compartments. Theoretically, these compartments are similar to the one studied in RA. The exact number and naming of compartments is often pre-determined by the life cycle database used by the practitioner.

However, the currently proposed 'consensus' method for the ecotoxicological impacts in LCA (USEtox) calculates only an impact for the freshwater compartment (Rosenbaum et al, 2008; Huijbregts et al, 2010). At present, no available method is recommended to assess marine and terrestrial ecotoxicity (JRC-IES, 2011).

Mandatory physical-chemical parameters needed for RA and LCA

Table 2.2 provides an overview of the data used in the environmental fate calculations of LCA and RA. It indicates a large similarity between these data types.

Table 2.2: Mandatory physical-chemical parameters needed for RA and USEtox fate calculation (for organics; adapted from Huijbregts et al (2010) and ECETOC TRA and easyTRA)

Input parameter	USEtox	RA
Molecular weight	Mandatory	Mandatory
Partition coefficient octanol-water	Mandatory	Mandatory
Vapour pressure	Mandatory	Mandatory
Water solubility	Mandatory	Mandatory
Degradation rate in air	Mandatory	Needed; can be modelled by the tool (based on standard degradation test data) if not available.
Degradation rate in water	Mandatory	Needed; can be modelled by the tool if not available.
Degradation rate in sediment	Mandatory	Needed; can be modelled by the tool if not available.
Degradation rate in soil	Mandatory	Needed; can be modelled by the tool if not available.

The use of single-species ecotoxicity data is another commonality between the two methods. These ecotoxicity data are used in lower tier RA to derive predicted no effect concentrations as threshold values. LCA uses the same type of experimental data to deduce the effect factors (see 3.1.2).
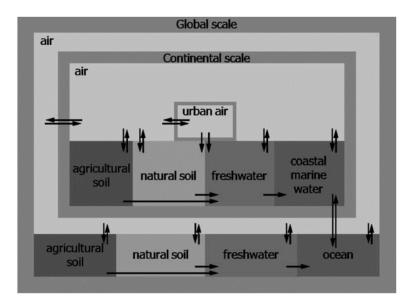
In addition, both assessments require information on the emissions of chemicals, i.e. the amounts and the compartments into which the chemicals are emitted. In RA this information is typically collected per life-cycle step. In LCA this information reflects the entire life cycle of a product or service. For efficiency reasons, assessors typically use data as provided via the life-cycle inventory databases.
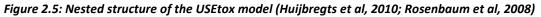
Approximating impact

The exposure assessment is complemented with an effect assessment yielding the effect factor EF in LCA or predicted no effect concentrations in ERA. In this regard, the use of (multiple) single-species ecotoxicity data is another commonality between the two methods. These ecotoxicity data are used in lower tier RA to derive predicted no effect concentrations as threshold values. LCA uses the same type of experimental data to deduce the effect factors (see 3.1.2). In the derivation of effect factors (LCA) or PNECs (RA), data from chronic ecotoxicity experiments can be used and assessment factors applied. However, the commonality is that single species laboratory data are used as a basis for the assessment. The resulting RCR or CF for an individual substance is assumed to reflect the impact on an entire ecosystem.
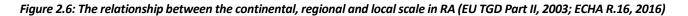
Mass balance based box models
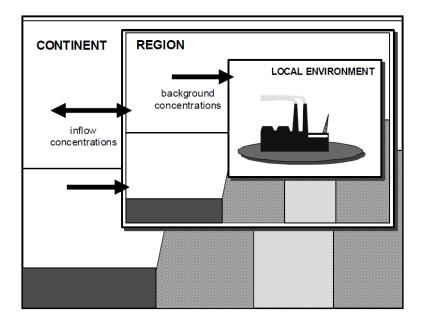
The USEtox impact method is based on an underlying multi-media fate model with nested compartments to account for distribution processes within, to and from the different nested regions (Figure 2.5; Huijbregts et al, 2010; Rosenbaum et al, 2008).

Figure 2.5: Nested structure of the USEtox model (Huijbregts et al, 2010; Rosenbaum et al, 2008)

Although RA is primarily performed on a local scale, the distribution processes take additional spatial scales into consideration, i.e. the local assessment receives a background concentration from the regional scale, and the regional scale receives the inflowing air and water from the continental scale (Figure 2.6; EU TGD Part II, 2003; ECHA R.16, 2016). This process is very similar to the nested structure of the USEtox model.

Figure 2.6: The relationship between the continental, regional and local scale in RA (EU TGD Part II, 2003; ECHA R.16, 2016)

The different calculation tools used in RA in the EU are all based on the EUSES Model (e.g. EUSES, ECETOC TRA, easyTRA) but differ mostly in their interface and user-friendliness. Their main task is the calculation of the PECs. As a prerequisite for this calculation, the tools need specific physical-chemical input parameters to correctly mass-balance the compound's partitioning in the environment. This is similar to USEtox which integrates a fate factor, an exposure factor, and an effect factor. Both the fate and the exposure factors are

derived by mass balance equations that describe processes such as degradation and inter-compartment transfer (Huijbregts et al, 2010). As outlined in 2.5.1 [Mandatory physical-chemical parameters needed for RA and LCA] the same physical-chemical input parameters as in the respective RA tools are needed. Table 2.2 lists mandatory physical-chemical input parameters for USEtox and RA.

In summary, it can thus be concluded that there is large methodological overlap in the derivation of values of CF for individual substance in LCA and in deriving RCRs in environmental RA. The substance property input data for exposure assessment and the exposure assessment methodology are identical. Even though effect characterisation differs by using PNEC in RA and EC_{50} in LCA, these effect metrics are based on the same experimental results.

Conclusion on methodological analogies

The assessment outputs of LCA and ERA are intended for different purposes, i.e. to quantitatively express the magnitude of an impact (in LCA) and to establish the proximity to a risk threshold (in ERA). However, the LCA assessment of a product is performed using very similar methodologies as a lower-tier risk assessment of a mixture. In both assessments, an exposure assessment is done. It consists of an emission assessment and of an environmental fate assessment.

Both assessments rely on a multimedia-fate model representing the environment as a system of nested boxes in order to account for the distribution of the chemical among compartments and from the source to distant environments.

The exposure assessment is complemented with an effect assessment yielding the ecotoxicity factor in LCA or predicted no effect concentrations in ERA. Depending on the LCA models, derivation can differ in the input data used (chronic and acute EC_{50}-data in USEtox vs NOEC (chronic) or acute EC_{50} data for ERA), assessment factors (one factor for acute to chronic extrapolation in USEtox as compared to multiple factors to account for data scarcity) and using geometric means in USEtox versus using the worst case data in ERA. The similarity is however, that single species laboratory data are used as a basis for the assessment and that for assessing the mixture additivity of the effects is assumed. With regard to ERA, the latter is true for lower tier assessment.

2.5.2   RA and LCA: Discrepancies

Objectives and General Approach

The main differences between LCA and RA are listed in Table 2.3. Both methodologies were designed to fulfil different objectives and can therefore not replace each other. However, they both can be used to guide the reduction of chemical impact on the environment. The main difference is that (environmental) RA typically addresses a single use situation of a single substance. In contrast, LCA attempts to assess the ecotoxicity impact of a functional unit (e.g. 1000 km of car travel, washing a wash load of laundry) covering all emissions occurring along the life-cycle.

Table 2.3: Summary of the main differences between LCA and RA (adapted from Olsen et al, 2001)

	LCA	RA
Aim – General	Compare / hotspot identification	Inform about safe use of chemicals
Objective – Ecotoxicity	Quantify ecotoxic impact	Establish need for risk management
Object of assessment / Scope	A functional unit - Emissions of all substances related to the entire life cycle of a product or service.	The single use of a single chemical
Result	Score - numerical expression for quantifying impact	Risk characterisation ratio – numerical expression of the comparison of chemical exposure versus the environmental effect threshold
Statement	Typically relative to alternative options	Absolute
Geography/ Temporality	Generic unit environment – not reflecting a specific situation in time and space. Not explicit in time and space.	Lower tier assessment of industrial chemicals: not specific in time and space. Higher tier assessments can be more specific.
Scale	functional units	Risk characterisation ratio (or Global production and use?) for actual emission volumes
Strategy for efficiency in assessment	Use of partial emission inventories from databases for establishing emission inventory for the functional unit (see 2.4)	Tiered approach: Start assessment with low-level data, refine if needed.
Dealing with uncertainty of data / results	Uncertainties are not explicitly addressed.	Apply safety factors to low-level data with safety factors, safety factors are reduced when refined data are used, refine input data when needed.

Assessment Objective

LCA aims at approximating the ecotoxicity impact of the chemicals which are emitted along all life cycle steps of a functional unit. Hence, LCA has to attempt to be accurate. On the other hand, the purpose of environmental RA of chemicals is to establish whether risk management is needed in order to avoid the unacceptable environmental impact of chemicals. To that end, single substances are assessed with regard to their hazard potential and their use. Chemicals cannot enter the market if they are not shown to be safe. Therefore, RA works as an absolute system with trigger or threshold values that must not be exceeded. The outcome of the assessment is the risk characterisation ratio (RCR) for each environmental compartment. It is the ratio of the predicted environmental concentration (PEC) and the predicted no-effect concentration (PNEC) which is derived from the experimental data applying an appropriate assessment/safety factor (EU TGD Part II, 2003; ECHA R.16, 2016). Under REACH the RCRs have to be below one to demonstrate that risks are controlled for a given use, and only chemicals with demonstrated safe uses are allowed to enter the market. The assessment has to be conducted for all lifecycle stages from the production of the substance down to the single downstream uses.

Estimation emissions

As a result, in the framework of LCA, emissions of chemicals that occur at any stage of the Life Cycle need to be accounted for. These emissions are associated with so-called 'foreground' (i.e. under your influence) and 'background systems' (not under your direct influence). For 'down-the-drain' products, such as cosmetics and

household products, the chemicals emitted to the environment are mainly related to the 'end of life 'stage (waste water treatment and solid waste handling), after which the residual chemicals are released to the natural environment. The environmental fate and (multimedia) exposure models used in ERA and LCA are overall very similar. However, emissions from other stages such as precursor and raw material production can sometimes play a significant role in the emission balance. In ERA, these emissions would be subject to different assessments, since they occur at different locations and moments. In LCA, they are all added up to reflect the emissions associated with the functional unit. In other words, there is no requirement for time- and geographical consistency/uniformity in LCA. This represents a very fundamental difference with ERA, where the whole method is focusing on calculating environmental levels that can be compared to so-called 'no-effect concentrations' (see Chapter 3). It is possible to experimentally validate a risk assessment, whereas it is impossible to experimentally validate an LCA.

Assessing single vs multiple substances

As LCA attempts to assess the ecotoxicity impact of a functional unit along the entire life-cycle, it has to address the ecotoxicity impact of multiple chemicals. As stated above, the ecotoxicity score in LCA is obtained by addition of the impacts of all chemicals emitted (NB: Impact = chemical emission x Characterisation Factor (CF)). In ERA, however, the additivity of chemicals is usually not attempted, and when it is done, grouping chemicals by the mode of action is considered to be the most correct approach. However, this approach is considered appropriate as a first tier risk assessment (ECETOC, 2011).

Ecotoxicity Data as Input for Reference Value Derivation

Ecological risk assessment and the USEtox methodology differ in the toxicity reference data used. In ecological risk assessment, PNEC-values are the reference for assessment. They are derived based on ecotoxicity data for the most susceptible trophic level. In contrast, the ecotoxicity factor used in USEtox can be based on chronic EC_{50}-data. In addition, the median, for instance, uses chronic EC/LC_{50} values as input parameters which are endpoint values not generally derived in experimental studies. Instead, these values need to be extrapolated from NOEC values or acute EC/LC_{50} values. This extrapolation introduces another uncertainty in the subsequent modelling which could be avoided if chronic NOEC or EC_{10} values were used from the beginning (without extrapolation) which are regularly derived from the respective chronic experimental studies and do not need to be extrapolated. If available, EC_{10} values are to be preferred as these values are usually obtained by regression analyses that take the whole concentration-effect relationship into account (ECHA R.10, 2008).

Extrapolation in Reference Value Derivation

If chronic data are not available, then it would be desirable to use acute EC/LC_{50} values for the assessment without further extrapolation. An alternative to acute EC/LC_{50} values would be deriving the chronic NOEC by applying the acute-to-chronic ratio concept. This concept is already applied in USEtox, however, the factor which is used is always 2 (10 for metals) regardless of the chemical class and the mode of action of the compound. To get a better approximation of the chronic toxicity a more precise acute-to-chronic ratio is recommended as outlined in ECETOC's Technical Report No. 91 (ECETOC, 2003). Another possibility to derive

chronic EC$_{50}$ values is a complete re-evaluation of the raw data of the experimental study itself. If the raw data are available and the study design allows the derivation of a chronic EC$_{50}$ value this would be an option to derive a scientifically sound value without the need to extrapolate from acute data. In LCA, it is also not uncommon to use QSAR data to fill data gaps for chemicals. Data of different quality and 'information' content are readily mixed in LCA, which is an important source of error and bias. This issue exists less in RA, where credit is given to (assumed) data quality via 'assessment factors', and where Klimisch-scoring of studies is routinely applied. In principle, those approaches could also find their way to the world of LCA.

It is also not clear how substances without any toxic effects are dealt with in LCIA. Consequently, these compounds should be excluded because the required input parameters cannot be derived. The natural variation of experimental data and the resulting consequences for RA and LCIA should also be taken into account.

Managing Data availability / quality

As the last aspect the availability and quality of the data used for LCA and included in the USEtox model need to be discussed. Since the enforcement of REACH in 2006, a huge amount of new experimental toxicity data has been generated for the ongoing REACH registrations. Furthermore, the already available data was re-evaluated according to current scientific knowledge. As a consequence, these evaluations and newly generated experimental data must be considered in LCA approaches and especially in the USEtox model. It goes without saying that the data used in LCA (as well as in RA) need to be regularly updated to be in line with the current scientific knowledge (as it is done in COsmede and AIIDA databases).

For registration purposes under REACH, acute and/or chronic aquatic toxicity data must be submitted in the registration dossier. These data are the basis for the subsequent ecological RA and are used for the derivation of the PNECs. Depending on the amount and quality of the data the PNECs are derived by applying an appropriate assessment factor to account for (1) intra- and inter-laboratory variation of toxicity data, (2) intra- and inter-species variations (biological variance), (3) short-term to long-term toxicity extrapolation, and (4) laboratory data to field impact extrapolation. These variations are inherent to the respective test system and cannot be avoided. For the use in RA the uncertainty resulting from these variations is compensated by the use of an appropriate assessment factor. A conservative approach is reasonable and supports the intention of RA to assure that the intended uses of the compound are safe. However, in LCA the goal is not safety but can be a comparison between different products. This approach is much more sensitive to any kind of uncertainty that might corrupt the overall outcome of the final comparison.

Strategies for Efficiency in Assessments

Efficiency in LCA is obtained by building the inventory of the functional unit to be assessed from partial inventories which can be obtained from LCI databases (e.g. EcoInvent, LCID). The rationale for this is that it is practically impossible to collect all the information on the material flows LCIs and the corresponding CFs along the life cycle for each assessment. Hence, the accuracy / uncertainty of the LCA ecotoxicity result is dependent on the data quality of the partial inventories in the LCI databases.

In order to be resource efficient, environmental RAs are performed in a tiered manner. In order to avoid 'false negatives' even with limited data sets, conservative default values and lower tier data (in combination with high safety factors) are applied in a first step. These yield a first approximation of the environmental impact. If PEC exceeds PNEC, the input values can be refined in order to obtain more realistic results. However, the RCR is always dependent on the specific input parameters and the risk management measures. Depending on these parameters, the value of RCR can differ and is thus neither suitable for a ranking nor a comparison between single substances.

Conclusions – Discrepancies

Threshold versus no threshold: ERA is based on the paradigm that there exists a concentration below which there is no effect of a chemical on the environment. Concentrations below the threshold are neglected (i.e. 'safe is safe'). In LCA, all emissions, even minuscule, are added in an attempt to calculate the overall 'chemical pressure' on the environment. In this context 'less is better'.

Dealing with missing data: In ERA, there is an incentive to generate more, and higher tier data, through the mechanism of decreasing assessment factors with increasing data richness. In LCA, by contrast, the absence of data will be 'beneficial' by keeping the impact score low. This is a critical practical shortcoming of LCA that, for the sake of comparability of results, needs to be addressed by agreements on product category rules and minimum data quality requirements.

Interpretation of results: in ERA, the probability of the risk occurring can be inferred from the RCR (Risk Characterisation Ratio), with low ratios being associated with low probabilities of occurrence in the real world. For RCRs above 1, however, it is difficult to impossible to predict the magnitude of the ecosystem impact. In LCA (USEtox method), the score (CTUe) reflects, to some extent, the expected ecosystem damage, but lacks the possibility to validate it further.

3. FRESHWATER ECOTOXICITY METHODS USED IN THE SUSTAINABILITY CONTEXT

This chapter gives an outline of the USEtox and the Critical Dilution Volume methodologies, two LCA methods commonly used to assess the aquatic impact of chemical-based consumer products, and briefly sketches additional assessment methodologies which are used to assess either risk or impact of chemicals or products containing chemicals.

3.1 USEtox Aquatic Ecotoxicity Model

USEtox is a multi-compartment environmental modelling tool that was developed to compare, via LCA, the impacts of chemical substances on ecosystems and on human health via the environment. It was developed by a group of scientists (modelling specialists) within the framework of the joint project 'SETAC-UNEP LCA Initiative'.

3.1.1 Brief historic overview

The USEtox model was developed between 2002 and 2009. Developers of other models such as CalTOX, IMPACT 2002 and USES-LCA were involved in the project (Medyna and Boyano, 2014). This consensual model was published in 2008 by Rosenbaum *et al* and launched officially in 2010 (USEtox v1.01).

An updated version of the model (USEtox v2.0) was published in 2015 including new or updated chemical parameters specific to substances. (e.g. pKa and partitioning coefficients were updated for organic and inorganic substances) (Huijbregts *et al,* 2015a; 2015c).

3.1.2 How does the USEtox model work?

As described by Medyna and Boyano (2014), "*USEtox models ecotoxicity impacts through the simulation of the release of chemicals by the technosphere, i.e. a manufacturing facility or a wastewater treatment plant, to the environment through mass flows between a succession of homogenous compartments. Overall the model distinguishes between emissions in six main urban and continental environmental compartments.*"

More precisely, USEtox method integrates three different types of emissions referring to six environmental compartments:

- Emissions to the air (Urban or Continental Air);
- Emissions to water (Freshwater or Seawater);
- Emissions to soils (Agricultural or Natural soils).

These compartments are assumed to be homogeneous for calculations.

In USEtox, the final impact of a product is expressed through an impact score (IS) that takes into account the characterisation factor (CF) of each ingoing substance as well as its mass as follows:

$$IS = \sum_x \sum_i CF_{i,x} \cdot M_{i,x} \tag{4}$$

Where:

$CF_{x,i}$ is the characterisation factor of the substance i released to the compartment x (CTUe/kg);
$M_{x,i}$ is the emitted mass of substance i to the compartment x (kg/d).

The CF of a substance represents the potential damage that the substance can cause in a specific compartment. Such a CF is expressed in comparative toxic units (CTUs), which correspond to the potentially affected fraction of species (PAF) per cubic meter per day per kilogramme emitted [PAF.m^3.day.kg$^{-1}_{emitted}$]. (Medyna and Boyano, 2014).

Hence, according to equation (4) the impact score is derived as the sum of all incremental impacts of the individual substances I resulting from their emissions M to air, water, and soil. The underlying assumption is thus that each chemical causes a substance-specific increment in species extinction and increments of species extinction can be summed up to yield IS as the overall species extinction. Hence, the resulting score addresses the entire mixture of chemicals which results from all chemical emissions related to a product or service, typically along the entire life-cycle.

When considering the global Life Cycle of a product, many flows appear. The Production phase of the product generally involves a high number of substances (*e.g.* pesticides for some chemicals of renewable origin) which are partly released in soil, water and sometimes in air. Then the Manufacturing phase also generates effluents which end up for example in water compartments. The Use stage most of the time induces emissions whose ecotoxicity can be assessed through the End-of-Life phase of the product.

Consequently, for a given product, different flows are generated during the whole Life Cycle and can be released either in one compartment of the environment or in several ones.

Figure 3.1 illustrates the modelling structure of an LCA environmental model. The blue rectangle shows the environmental model boundaries and the red rectangles the current freshwater ecotoxicity model boundaries of USEtox.
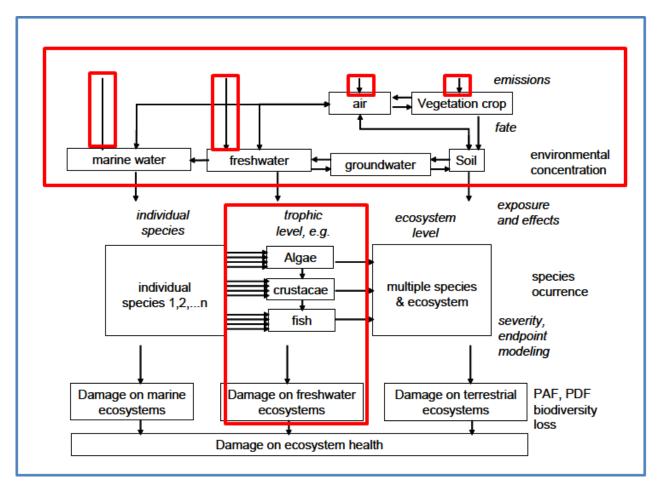
Figure 3.1: Flow diagram for ecotoxicity (adopted from JRC-IES, 2011). Red rectangles were added to illustrate USEtox method boundaries

Transfers between compartments and toxicity effects are accounted for by the CF. Indeed, CF (which are implemented in USEtox model) are calculated based on three factors as follows (Rosenbaum *et al*, 2008):

$$CF = FF \times XF \times EF \qquad (5)$$

Where (for freshwater ecotoxicity):

FF is the fate factor of the substance considered, expressed in days (d);

XF, its exposure factor (dimensionless);

EF, the effect factor expressed in PAF m^3.kg^{-1}.

Fate factor

The repartitioning of emissions in the environment for a given substance must be known or estimated to apply the right USEtox CF. This is achieved via the fate factor (FF). Besides repartitioning, it expresses the time a substance persists in an environmental compartment. More precisely, this factor describes the behaviour of a substance released in the environment, taking into account removal processes (e.g. degradation by

microorganisms, burial into sediments, leaching to groundwater, escape to the stratosphere) and intermedia transports between compartments (advective or diffusive transport).

FF calculation requires a least eight parameters for organics and six parameters for metals and inorganics (Medyna and Boyano, 2014), such as degradation rates in the different compartments or partitioning coefficient.

Exposure factor

The exposure factor (XF) represents the fraction of a substance which is dissolved in freshwater and thus available for freshwater species (bioavailability). This factor is needed to take into account that only a part of the substance which finally persists in freshwater is available to induce toxic effects. Bioavailability considerations are also very important for metal exposure and effects modelling.

Data gathered for FF calculation are also used to calculate XF.

Effect factor

The EF for the aquatic environment is defined as

$$EF = \frac{0.5}{HC50_{EC50}} \qquad (6)$$

In equation (6) HC_{50} is calculated as the geometric mean of the EC_{50} values measured in different species.

The EF for the aquatic environment reflects the change in the potentially affected fraction of species due to exposure to the substance. In this sense, it is some form of biodiversity indicator.

EF calculation is based on a geometric mean of hazardous concentrations measured or estimated for different species. More precisely, EF is calculated from an HC_{50} (in mg/L). As defined in Rosenbaum et al (2008), HC_{50} is "the hazardous concentration at which 50% of the species are exposed above their EC_{50}", considering that "The EC_{50} is the effective concentration at which 50% of a population displays an effect (e.g. mortality).

In the USEtox model, two types of EC_{50} values can be applied: chronic and acute EC_{50} values. Chronic values refer to a long-term lethal toxicity while acute values correspond to a short-term lethal toxicity. Chronic EC_{50} values are prioritised to calculate the HC_{50}. Otherwise, acute EC_{50} values are used. Acute EC_{50} values are converted into chronic EC_{50} values by applying an extrapolation factor of 2 for organic substances. Specific extrapolation factors have to be applied for cationic metals (Huijbregts *et al,* 2015b).

If any one species has several EC_{50} values (resulting from different measurements or tests), the EC_{50} value of this species used to calculate the HC_{50} is the geometric mean of the available EC_{50} values.

As mentioned before, the chronic EC_{50} endpoint values are only rarely reported in existing study reports, because in the past it did not serve any particular evaluation purpose. Also, in chronic tests several endpoints

besides mortality can be evaluated and can lead to an NOEC or EC_{10} value, while the reported EC_{50} would typically be based on mortality.

Reference data

In USEtox databases, *Recommended* data/CF and *Interim* data/CF are distinguished. This distinction reflects the "*level of expected reliability of the calculations in a qualitative way*" (Rosenbaum *et al,* 2008).

Moreover "*It should be stressed that the characterisation factors are useful for a first tier assessment. In case a substance appears to dominantly contribute to the impact scores for toxicity, it is recommended to verify the reliability of the chemical-specific input data for this substance and to improve the data whenever possible*" (Huijbregts *et al*, 2015b).

For those substances not found in the USEtox databases, it remains possible for the user to calculate a CF by means of the USEtox model (via an Excel-based tool) when the appropriate data set is available.

3.1.3   Key points and limitations

Since its launch in 2010, the USEtox model has evolved. More CFs are now available. Data for inorganics have been improved. However, the relevance of this method and uncertainty on the results remain a subject of debate. Table 3.1 lists major advantages and limitations of USEtox.

Table 3.1: Advantages and limitations of USEtox

Advantages	Limitations
Consensual LCA model recommended in the PEF Guide: it is implemented in most of the LCA softwares such as SimaPro, OpenLCA,… Multi-compartment model: the fate factor (FF) integrates different compartments were substances can be retained or degraded. More than 3000 CFs are already available from the developers and the number is increasing.	USEtox method is relevant to identify hotspots in Life Cycle. However at least two orders of magnitude are needed to differentiate freshwater ecotoxicity results due to uncertainty (Rosenbaum et al, 2008), which means it is not precise enough for comparison between 'similar' substances or products. The effect part (EF) is based on a geometric mean of chronic aquatic (lethal) EC_{50} for all species confounded. USEtox thus takes into account neither variation in sensitivity of the different trophic levels, nor species that are most sensitive to the effects of some substances (e.g. cationic substances). So any disturbance in trophic chains cannot be assessed. Numerous data are needed to calculate one CF. Time spent to calculate is non-negligible (typically several hours per substance for data collection and review, depending on available information).

3.2 Critical Dilution Volume model

3.2.1 Brief historic overview

In a method for Environmental LCA of products published in 1992 (Heijungs *et al*, 1992), impacts on aquatic ecosystems were assessed by means of an Ecotoxicological Classification factor for Aquatic ecosystems (ECA) expressed in m^3 water.kg^{-1} of substance. This indicator is considered as the origin of the CDV method.

The CDV approach was developed in 1995 to provide the first EU Ecolabel for laundry detergents. The CDV method was revised in 2004 as well as the Detergent Ingredient Database (DID) list. This list was then updated in 2007 and 2014. The CDV result is now a key criterion in the two EU Ecolabels for detergents (EC, 2013b) and rinse-off cosmetic products (EC, 2014a), in the Nordic Ecolabels (Nordic Ecolabelling, 2010; 2013) and in the French *Standard NF Environnement* (AFNOR Certification, 2011).

3.2.2 How does it work?

The CDV method estimates an impact on aquatic freshwater ecosystems through a volume of natural water required to dilute a quantity of product (or functional unit) down to a concentration without any foreseeable harmful impact on aquatic species.

Unlike USEtox, the CDV method only considers direct emissions to freshwater (e.g. emissions to the air with potential impacts on freshwater species are not taken into account). Boundaries are thus restrained to emissions to the freshwater compartment only. These boundaries are illustrated bellow with orange rectangles added in Figure 3.2.
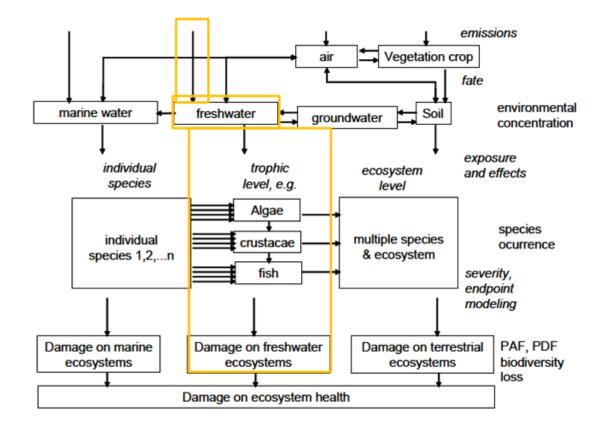
Figure 3.2: Flow diagram for ecotoxicity (JRC-IES, 2011). Orange rectangles were added to illustrate CDV method boundaries

The calculation of CDV is based on substances flows multiplied by characterisation coefficients. Final impact of a product is assessed as follows (Gleerup Ovesen *et al*, 2013):

$$CDV = \sum_i Dose_i \times 1000 \times \frac{DF_i}{TF_i} \qquad (7)$$

Where:

Dose$_i$ is the mass of substance i per recommended dose or per quantity of active content. It is expressed in g/dose (equivalent to g/functional unit) (European Ecolabel, 2011) or in g/g of active content (equivalent to the sum of organic ingoing substances in the product) (EC, 2014a).

DF$_i$ is the degradation factor for ingredient i.

TF$_i$ is the chronic toxicity factor of the ingredient i (in mg/L).

The CDV may be expressed in L/ dose or in L/g of active content.

Degradation factor (DF):

DF is an estimation of the degradation rate of a substance in the aquatic environment. It results from tests assessing aerobic biodegradability (Test methods 301 A to F or 310 in the OECD Guidelines for the Testing of Chemicals).

Even if DF are supposed to represent degradation rates in natural freshwater, kinetics show similarities with biodegradation of substances in wastewater treatment plants.

Actually, DF are fixed and fall in one of the five 'bins' (Gleerup Ovesen *et al*, 2013) presented in Table 3.2. It reflects the fraction left after application of the fate process.

Table 3.2: DF values according to the biodegradation potential

Category	Degradation factor, DF
Instant degradation	0.01
Readily biodegradable	0.05
Readily biodegradable failing 10-d window	0.15
Inherently biodegradable	0.5
Persistent	1

Finally, DF is an equivalent to the fate factor in USEtox model. However, it takes neither transfer between environmental compartments nor removal processes other than biodegradation into account. This coefficient represents therefore a very simplistic tool to model the fate of ingredients in the freshwater compartment. A former version of the DF, named Loading Factor (LF), included a sorption criteria based on the n-octanol/water partition coefficient (Kow) (Eskeland and Svanes, 2004; Nitschke *et al*, 2007). According to the authors, calculations with this former DF take into account the biodegradation potential and the adsorption capacities of substances to suspended particles and sludge in a wastewater treatment plant. Considering that sludge may be used as fertiliser, resulting in a second potential pollution, it was then decided to remove adsorption from LF and to keep only biodegradability in CDV equations (European Ecolabel, 2011).

Consequently, the resulting DF is overall easier to calculate than the USEtox fate factor.

Toxicity Factor (TF):

TF is calculated by dividing aquatic toxicity (either NOEC, EC_{10}, $EC_{50,}$ or LC_{50}) by a safety factor (SF). So aquatic toxicity data are not aggregated and used in the same way to determine TF in CDV method and EF in the USEtox method.

The CDV method compares values obtained for each one of the three standard trophic levels studied (fish, crustaceans and algae). When data on different species belonging to the same trophic level are available, a median value is calculated. This median is considered to be the general response of species in this trophic

level and is compared to other trophic level (median) values (EC, 2014c). The lowest (median) value is then kept to determine the CDV result.

Chronic toxicity data (*e.g.* evaluating long term effects on studied populations) are preferred but when missing, acute data (*e.g.* assessing short term effects on studied populations) can also be used. In any case, a specific SF is applied depending on the data set available (measurements performed on the three trophic level species or less; chronic data available or not).

Table 3.3 shows the different SF to be applied depending on the situation (EC, 2014c).

Table 3.3: TF values according to the aquatic toxicity data set

Data	Safety factor (SF)	Toxicity factor (TF)
1 short-term L(E)C$_{50}$	10000	Toxicity/10000
2 short-term L(E)C$_{50}$ from species representing two trophic levels (fish and/or crustaceans and/or algae)	5000	Toxicity/5000
At least 1 short-term L(E)C$_{50}$ from each of three trophic levels of the base-set*	1000	Toxicity/1000
One long-term NOEC or EC$_{10}$ (fish or crustaceans)	100	Toxicity/100
Two long-term NOEC or EC$_{10}$ from species representing two trophic levels (fish and/or crustaceans and/or algae)	50	Toxicity/50
Long-term NOEC or EC$_{10}$ from at least three species (normally fish, crustaceans and algae) representing three trophic levels	10	Toxicity/10

*The base set for testing the toxicity of substances towards aquatic organisms consists of acute tests with fish, *daphnia* and *algae*.

Reference data:

To date, TF and DF have been assigned to about 200 ingredients, in particular for those used in for cleaning products. These results are summarised in the last version of the Detergents Ingredients Database (EC, 2014b).

Current data mostly derive from acute toxicity, as chronic data were not often available. Most TF thus include a high SF.

For those ingredients not found in the DID-list Part A, the DID List Part B (2014c) gives the methodology to determine the DF and TF.

3.2.3   Key points and limits

As for the USEtox model, the CDV method also has advantages and limits. These are summarised in Table 3.4. The CDV method is one of the key criteria to award a Nordic or European Union (EU) ecolabel to detergent and cosmetic products (EC, 2014a; Nordic Ecolabelling, 2010). It corresponds to a Midpoint indicator. The environmental scope of the CDV method is the same (freshwater impact) as the USEtox ecotoxicity. Both USEtox and CDV assume additivity of ecotoxicity of the formula constituents. They do not take into account the chemical constituent mode of action and possible interactions (*e.g.* synergisms, antagonisms…), which could take place in the environment.

Table 3.4: Advantages and limits of CDV

Advantages	Limits
CDV has been chosen as the reference model in European and Nordic Ecolabels	Mono-compartment model.
Easy to apply thanks to a limited number of data needed. It is thus an efficient tool to help improving the environmental profile of products based on key parameters (biodegradability and aquatic toxicity).	The available fraction of constituents in freshwater is overestimated as adsorption potential of these constituents on suspended particles or sediment is not taken into account.
	Result uncertainty of this method has not been assessed yet.
The ecotoxicity part (TF) is ecologically relevant. It considers the most sensitive trophic level and thus prevents theoretically from any disturbance in trophic chains.	In the CDV method for cosmetic rinse-off products, the volume of water is expressed per gram of organic matter of product, although it would be wiser to express it per gram of formula or dose/functional unit.
Adsorption of substances on suspended particles or sediment is not taken into account, but assuming 100% behaviour in the water phase is consistent with the precautionary principle.	At present the CDV database is not developed enough to take into account all phases of an LCA (about 200 ingredients are found in the DID list part A covering end-of-life stage of a limited number of substances found mainly in detergents and cosmetics.

3.2.4   USEtox and the Critical Dilution Volume method

CDV is the method currently employed in the EU ecolabel to detergent and cosmetic products (EC, 2014a; Nordic Ecolabelling, 2010). Currently it is not used within the LCA community since it is not available in the common LCA databases. This could be changed, however, with not too much effort by databases providers. Both models can be used to score impact on the aquatic ecosystem, but differ in the approach and finally also the scope they currently cover. The most important differences are summarised in the following paragraphs.

Comparison of USEtox and CDV principles

USEtox and CDV were developed to provide tools in different contexts. That is why their operation and use differ. However, both are Midpoints indicators and can help assessing impacts of chemicals on freshwater aquatic ecosystems. Both are also limited by data availability and quality especially when considering the whole life cycle of a product.

As a conclusion, advantages and drawbacks of both methods are summarised in Table 3.5.

Table 3.5: Comparative analysis of USEtox and CDV relevance

Method	USEtox	CDV
Fate	Relevance : +++ →Emissions to air/soil/water considered →Multi-compartment fate modelling (but complex to calculate)	Relevance : + →Emissions to air and soil not considered →Mono-compartment fate modelling (but easy to calculate)
Freshwater toxicity	Relevance : + → Geometric mean based on all available species data → Extrapolation factors from acute to chronic EC_{50} inconsistent with regulatory method	Relevance : +++ →Most sensitive trophic level retained for calculation →Safety factors to determine TF from ecotoxicity data consistent with regulatory method (worst case scenario when data are missing)
User-friendliness	: + → more than 10 parameters per substance needed when CF not available	: ++ →2 parameters / ingredient needed → But limited number of ingredients in the DID-list Part A
PEF applicability	Relevance: + → Comparison of consumer products limited by results uncertainty	Relevance: ++ → Comparison of consumer products based on 2 key environmental parameters (biodegradation and aquatic ecotoxicity) assuming results uncertainty reduction with the number of parameters needed

The following chapter of this document presents results of a case study aiming to compare results from USEtox and CDV methods with a virtual formula.

Fate modelling

USEtox employs a multi-compartment fate model that allows emissions to receiving compartments air/water/soil to re-distribute. This fate model reflects transfers that occur in the environment between the different environmental compartments. However, some data required by this model are difficult to collect. This may limit the number of substances that are parametrized or result in introducing modelling or default data for some parametrized substances.

In CDV emissions to air and soil cannot currently be considered, thus resulting in a less complete fate modelling. However, the fate model in CDV allows a very facile parametrization and thus calculation.

Freshwater toxicity calculation

Theoretically CDV and USEtox methods can use the same data set to calculate their respective ecotoxicity factors.

In USEtox, a geometric mean based on all available ecotoxicity data is used to assess freshwater toxicity because this approach is considered more statistically robust to derive the effect factor.

In CDV, the most sensitive trophic level is retained for the calculation of the effect factor. This method considers that impacting at least one trophic level of a given ecosystem can disturb the whole ecosystem functioning. This way to derive the effect factor appears to be more environmentally realistic.

Use of the methods

CDV is simple to apply since only two parameters are required per substance, compared to the much higher number of parameters needed in USEtox. Currently, however, the CDV method is geared towards the use in detergents and cosmetics, so the parameters are readily available from the so called DID list (see § 3.2.2) for a limited number of chemicals. For all other cases the parameters will have to be generated, which is expected to be a lesser burden compared to the number of parameters required by USEtox.

Applicability in PEF

CDV is simple to apply for comparison of down-the drain consumer products in the range of cosmetics and laundry detergents based on the 2 key environmental parameters (biodegradation and aquatic ecotoxicity) required and the fact that for many ingredients the parameters are already tabulated. Assuming that uncertainty increases with the number of parameters needed, CDV compares favourably with USEtox, but is limited in scope to direct emissions into water due to the missing fate-model.

3.3 Additional Ecological Risk / Impact Assessment Methods

3.3.1 A.I.S.E. ESC

The Environmental Safety Check (ESC) is a tool to assess cleaning product formulations for their safety towards organisms living in the aquatic environment (Pickup et al, 2016). The method is developed as part of a sustainability evaluation scheme for cleaning products in EU, i.e. the AISE charter for sustainable cleaning. It applies a conservative, but tiered evaluation approach considering environmental data and estimation of ingredient volumes in the market. Products that qualify for a variety of AISE charter sustainability criteria, including the ESC are allowed to use the AISE charter company and product logo. To qualify for ESC, companies need to do due diligence on their formulations and substances, thereby respecting the specific rules of the approach. The primary driver for developing ESC was to provide a product-specific assessment and assurance of safety in response to stakeholder demands, as REACH operates at ingredient / substance level. Although risk assessment at ingredient level is adequate to assure environmental safety, product-level assessment is potentially complementary in guiding sustainable development, and providing a basis for product-specific safety assurance for the consumer. This is implemented through a simple spreadsheet tool and internal database of ingredient parameters including PNEC (predicted no-effect concentration) and removal rate. A novel feature is applying market volume information at the level of both the product types and the ingredients, to permit a realistic risk-based calculation. To pass the ESC check the PESR (projected environmental safety ratio) for each ingredient as formulated and dosed must be less than 1.

3.3.2   ProScale

ProScale is a new approach to describe relative potential toxicological performances of products and allow for comparisons with other products related to a defined functional unit in an LCA context. ProScale is intended to be used as additional information in the framework of LCA, more specifically in Environmental Product Declarations (EPDs) and PEF, with a first focus on human toxicity impacts but with the possible extension to ecotoxicity and other product groups.

ProScale was first outlined in 2015 by Fritz Kalberlah (FoBIG), Eva Schmincke (thinkstep) and Birgit Grahl (Integrahl) in a study commissioned by BASF with the idea of proposing a performance based indicator using REACH data in the LCA framework. After having been presented to several stakeholders, ProScale is further developed by a consortium that intends to publish results in 2017. ProScale main characteristics are:

1) It starts from the products ingredients and considers the substances in their different life cycle stages.

2) It combines information on hazard and exposure for each substance and each life cycle stage, by combining a factor describing the hazard with a factor describing the exposure. Both factors are based on available data or tools, for example in the REACH context.

3) It allows aggregation on the different life cycle stages and of the different substances to the product level. Furthermore, life cycle steps of using the product in a specified application until the end-of life are intended to be considered in the assessment.

4. FRESHWATER ECOTOXICITY AS A SELECTIVE IMPACT CATEGORY: AN ILLUSTRATIVE CASE STUDY

A case study was conducted to discuss freshwater ecotoxicity as a relevant impact category to guide the selection of chemical-based products in the context of environmental performance. The case study aimed at analysing the environmental impact of a virtual 'down-the-drain' product at different stages of its life cycle, and especially focused on comparing the USEtox and CDV approaches in the assessment of downstream impact scores. The reader will find in this chapter an introduction to the system model and virtual product selected for the case study, a presentation of the materials and methods used for the calculation of the impact scores, and a descriptive overview of the results. The latter will be further discussed and analysed in Chapter 5.

4.1 Preamble

4.1.1 Model system boundaries

Life Cycle Assessment is flexible regarding the choice of system boundaries. For example, the life cycle of consumer products can often be cast in the schematic steps or stages as shown in Figure 4.1. Here, each arrow captures a step in the life cycle of a product. 'Raw materials' captures the impacts for creation and refinement of materials in the value chain extended upstream. 'Production' captures the operations of a consumer goods corporation that uses refined raw materials to manufacture their products. 'Logistics' captures inbound as well as outbound transport of raw materials and finished goods. 'Industrial processing or retailing' models handling by business customers, e.g. cooling of products in stores. 'Consumer use' refers to the application of the product by the end consumer. 'Disposal' captures the final stage after use of the product. For products used in conjunction with water, this often means disposal of the packaging in solid waste streams, whereas the liquid is typically subjected to municipal wastewater treatment.

Figure 4.1: Boundaries of the model system used in the case study

The eye illustration highlights the vantage point adopted in the case study. All life cycle steps to the left are termed 'upstream' whereas all life cycle steps to the right are termed 'downstream'.

A study covering the entire value chain from the creation of the raw materials (starting with extraction of the most basic raw materials from nature) over production, use and disposal is referred to as a cradle-to-grave assessment. To achieve the objective of this taskforce, we chose to use a reduced scope, including only two

life cycle stages in the study. These stages are the 'Raw materials' creation stage at the beginning of the value chain and the 'Disposal' stage at the end of the value chain. Our own vantage point is that of the producer of a virtual product and thus marked 'Production' (Figure 4.1). This reduced model thus does not have the objective of explaining in full detail the entire life cycle of an actual product, but to enable a focused study of the implications of modelling freshwater ecotoxicity in the LCA setting.

Our choice of system boundaries was rationalised by accounting for the fact that in LCA the environmental burden is carried onwards in a 'backpack' that gradually gains weight over the supply chain and entire value chain. As a part of a supply chain, one has to face the problem that the upstream contributions of raw material creation are often impossible to quantitate exactly. In a typical Life Cycle Assessment, this information is thus often modelled and approximated by datasets obtained from public or commercial databases. The same is often true for the downstream applications of a product. For some defined applications, however, e.g. cosmetic or laundry products, it is clear that a product is quantitatively subjected to the wastewater stream. In such a case the modelling of the 'Disposal' stage can be obtained with a lesser set of assumptions and unknowns, e.g. than imported by the 'Raw materials' stage from upstream. Since the modelling approach is very different and allows us to analyse the influence of life cycle based modelling assumptions on the results, both 'Raw materials' and 'Disposal' were included in the modelling. Please note that although we choose our vantage point to be at the production stage (please refer to Figure 4.1), this particular life cycle stage is a dummy only to explain the perspective adopted and does not contribute to the model with any emissions and thus impact. It is used here solely to illustrate the perspective adopted and the typical information sources and logic employed in modelling 'upstream' and 'downstream' in LCA. Any material emissions that would occur due to production would follow the same modelling approach as we apply to the disposal stage. Since we see the quantitative disposal of a product into wastewater as a kind of 'worst-case' scenario and is also highlighted as being of particular importance by currently running PEF pilot studies (e.g. for detergents products), we chose to look into the expected higher contribution of the disposal stage rather than production. Neither logistics nor retailing are expected to be of major significance and thus would only lead to higher complexity in assessment and discussion rather than to a clarification of the subject matter.

4.1.2 Virtual product specifications

A virtual product was set up to serve as an example for the calculation of freshwater ecotoxicity impact scores by the USEtox and CDV approaches. Its composition was established from the one of standard 'down-the-drain' consumer products (e.g. homecare/personal care products) and included in-going substances (= ingredients) usually found in cosmetic or detergent products (e.g. surfactants). Substances found in plant protection products (e.g. organic/inorganic biocides) were however also included in the composition of the product. The underlying rationale was to set up a virtual product representative of a wide range of fate and ecotoxic properties rather than to set up a product fit for use in a specific market area. In addition to their properties, in-going substances were also selected according to the availability in LCA and RA databases of the input data necessary for the calculation of impact scores. For example, substances for which no Unit Process Raw (UPR) data were available in LCA databases were not retained for inclusion in the virtual product.

4.2   Materials and methods

4.2.1   Composition of the virtual product

The virtual product was defined as an aqueous blend of linear alkylbenzene sulphonate (LAS), acetic acid, ethanol, zinc sulphate, benzisothiazolinone (BIT), acrylic acid and alachlor. The exact composition of the virtual product is reported in Table 4.1.

Table 4.1: Composition of the virtual product used in the case study

Substance name	CAS number	Molecular formula	Content (% w/w)
Linear alkylbenzene sulphonate (LAS)	68411-30-3	C16-19H25-31SO3.Na	5.00
Acetic acid	64-19-7	C2H4O2	5.00
Ethanol	64-17-5	C2H6O	5.00
Zinc sulphate	7733-02-0	SO4.Zn	1.00
Benzisothiazolinone (BIT)	2634-33-5	C7H5NOS	1.00
Acrylic acid	79-10-7	C3H4O2	0.10
Alachlor	15972-60-8	C14H20ClNO2	0.05
Water	//	//	Up to 100%

4.2.2   Calculation of the impact scores

As USEtox is a life-cycle based approach, it was an appropriate tool to assess the environmental impact of both the upstream 'Raw materials' and downstream 'Disposal' stages, especially as the databases linked to the model covers substances produced and/or emitted throughout the whole life-cycle. Two versions of the model were used: version 1.01 (released in February 2010) and version 2.0 (released in August 2015). Calculation of the impact scores for the 'Raw materials' stage was however only possible with the older version as for the newly released one, key UPR data were missing. Otherwise, although CDV was initially developed for environmental LCA, the database linked to it is currently limited to a set of *ca.* 600 substances mainly used in detergents. Data are thus missing to estimate the impact of all the substances produced and emitted during the production phase (i.e. upstream 'Raw materials' stage). Consequently, CDV was only used to assess the environmental impact of the downstream 'Disposal' stage. In the end, the USEtox approach was used to compare the relative contribution of each life cycle stage to the environmental impact of the virtual product, whereas the CDV approach was used to compare the environmental impact scores obtained with the USEtox approach for the downstream stage.

Upstream impact scores

The impact of the 'Raw materials' stage was calculated using the Ecoinvent 2.2 database in conjunction with USEtox 1.01 characterisation factors for freshwater ecotoxicity. As mentioned in *Chapter 2.2*, LCA databases such as Ecoinvent 2.2 provide aggregated datasets. The identification of the main impacts along the production chain requires the disaggregation of the datasets. In the case of our virtual product, the disaggregation of the datasets up to extraction of raw materials is very complex. Therefore, the impacts of the production chain were analysed focusing on one ingredient of the virtual product: LAS. The LAS tree, as shown in *Chapter 2.4*, was tracked back up to level 5, which was sufficient to identify the main impact contributors. In addition to the main production steps and processes, the disaggregation procedure also revealed the main substances and elements causing freshwater ecotoxicity. The results are thoroughly discussed in *Chapter 5*.

Downstream impact scores

- USEtox approach

The impact of the 'Disposal' stage was calculated using USEtox v1.01 and v2.0 characterisation factors for freshwater ecotoxicity. The input data used by both versions of the model to calculate the characterisation factor of each ingredient in the virtual product are presented in Table 4.2.a (USEtox v1.01) and Table 4.2.b (USEtox v2.0). The differences between the two input datasets are highlighted in the tables. Of note is that the Database Inorganics (USEtox v1.01, v2.0) contains data for metal elements but not for metal salts; for zinc sulphate, a CF had thus to be calculated first for zinc element and then to be expressed in zinc sulphate using a molar conversion factor of 0.4 (it was assumed that the sulphate counter-ion had no or little influence on the impact score of the whole salt).

Table 4.2: Input data used to calculate by the USEtox approach the downstream impact score of each ingoing substance identified in the virtual product

(a) USEtox v1.01 input data. Datasources: USEtox v1.01 – Database Organics, USEtox v1.01 – Database Inorganics.

Substance name	Kow (L.L⁻¹)	Koc (L.kg⁻¹)	K_H25 (Pa.m₃.mol⁻¹)	$P_{vap}25$ (Pa)	Sol25 (mg.L⁻¹)	kdeg$_A$ (s⁻¹)	kdeg$_W$ (s⁻¹)	kdeg$_{Sd}$ (s⁻¹)	Kdeg$_{Sl}$ (s⁻¹)	av$_{logEC50}$ (mg.L⁻¹)	BAF$_{fish}$ (L.kg$_{fish}$⁻¹)
LAS	104.71	3728.21	3.09E-12	1.71E-12	1.77E+02	1.00E-05	5.35E-07	5.94E-08	2.67E-07	0.65	3.16
Acetic acid	0.68	1.00	1.01E-02	2.09E+03	1.00E+06	5.55E-07	9.25E-07	1.03E-07	4.63E-07	2.06	3.16
Ethanol	0.49	1.58	5.05E-01	7.91E+03	1.00E+06	2.45E-06	9.25E-07	1.03E-07	4.63E-07	3.17	0.92
Zinc	No data	No data	1.00E-20	No data	No data	1.00E-20	1.00E-20	1.00E-20	1.00E-20	0.02	4700.00
BIT	4.37	34.47	2.42E-05	3.43E-03	2.14E+04	1.27E-05	5.35E-07	5.94E-08	2.67E-07	0.07	1.31
Acrylic acid	2.24	1.44	3.74E-02	5.29E+02	1.00E+06	7.29E-06	9.25E-07	1.03E-07	4.63E-07	1.46	3.16
Alachlor	3311.31	190.55	8.40E-04	2.73E-03	2.40E+02	3.38E-05	1.34E-07	1.49E-08	6.69E-08	-0.45	13.20

(b) USEtox v2.0 input data. Datasources: USEtox v2.0 – Database Organics. USEtox v2.0 – Database Inorganics.

Substance name	Kow (L.L⁻¹)	Koc (L.kg⁻¹)	K_H25 (Pa.m₃.mol⁻¹)	$P_{vap}25$ (Pa)	Sol25 (mg.L⁻¹)	kdeg$_A$ (s⁻¹)	kdeg$_W$ (s⁻¹)	kdeg$_{Sd}$ (s⁻¹)	Kdeg$_{Sl}$ (s⁻¹)	av$_{logEC50}$ (mg.L⁻¹)	BAF$_{fish}$ (L.kg$_{fish}$⁻¹)
LAS	104.71	No data*	3.09E-12	1.71E-12	1.77E+02	1.00E-05	5.35E-07	5.94E-08	2.67E-07	0.65	204.27*
Acetic acid	0.68	1.00	1.01E-02	2.09E+03	1.00E+06	5.55E-07	9.25E-07	1.03E-07	6.69E-06*	2.06	0.95*
Ethanol	0.49	1.58	5.05E-01	7.91E+03	1.00E+06	2.45E-06	9.25E-07	1.03E-07	4.63E-07	3.17	0.92
Zinc	No data	No data	1.00E-20	2.00E-11*	No data	1.00E-20	1.00E-20	1.00E-20	1.00E-20	-0.75*	4700.00
BIT	4.37	No data*	2.42E-05	3.43E-03	2.14E+04	1.27E-05	5.35E-07	5.94E-08	2.67E-07	0.07	1.31
Acrylic acid	2.24	No data*	3.74E-02	5.29E+02	1.00E+06	7.29E-06	9.25E-07	1.03E-07	4.63E-07	1.46	1.09*
Alachlor	3311.31	190.55	8.40E-04	2.73E-03	2.40E+02	3.38E-05	1.34E-07	1.49E-08	5.73E-07*	-0.45	13.20

*Input data different from the corresponding one used in USEtox v1.01.

- CDV approach

The CDV of the virtual product was calculated according to the formula reported below:

$$CDV = \sum_i weight_{(i)} \times CDV_{(i)} \qquad (8)$$

where:
- $weight_{(i)}$ is the weight of the ingoing substance *i* (in kilograms) per 1 kilogram of product;
- $CDV_{(i)}$ is the CDV of the ingoing substance *i*.

The CDV of each ingoing substance was initially calculated according to the formula reported in Chapter 3 (§3.1.2). The calculation followed the tiered-approach implemented in the European Union (EU) and the Nordic Ecolabelling Schemes for products disposed of 'down-the-drain', *e.g.* Rinse-off cosmetic products (EU, 2014; Nordic Ecolabelling, 2015). The CDV input parameters (*i.e.* Degradation Factor, DF; Toxicity Factor, TF) were taken where possible from the Detergents Ingredients Database (DID-list) Part A version 2014.1, the toxicity factors derived from long-term (TF$_{chronic}$) being always preferred over those derived from short-term data (TF$_{acute}$). For substances not listed on the DID-list Part A, TF and DF values were determined according to the procedure described in the DID-list Part B version 2014.

The toxicity factor TF is defined in the following manner: TF = toxicity/SF, where 'toxicity' designates the lowest median long-term NOEC or acute E(L)C$_{50}$ calculated over three trophic levels (fish, crustaceans and algae), and where the applied Safety Factor (SF) depends on the type/number of available data (cf. Table 3.2 in Chapter 3). The median value within each trophic level is calculated using validated test results and the lowest median of the trophic levels is used to determine the toxicity factor. If several results are available for one species within a trophic level, a median value is first calculated for the species and then used to calculate the median value for the trophic level; if no long-term NOEC value is available, acute E(L)C$_{50}$ values have to be used.

The degradation factor DF refers to degradation under aerobic conditions and is defined as the extent to which a substance is degraded before reaching the receiving waters (Gleerup Ovesen *et al*, 2014). For instance, an emission of 5% to the environment is assumed for readily biodegradable substances whereas an emission of 100% to the environment is assumed for persistent substances (cf. Table 3.1 in Chapter 3).

Among the substances identified within the virtual product, four are listed in the DID-list Part A: LAS (DID-list no. 2001), acetic acid (DID-list no. 2567), ethanol (DID-list no. 2529) and BIT (DID-list no. 2401). The TF and DF values used to calculate the CDV of those four substances were thus directly picked from the list. For substances not listed in the DID-list Part A, the TF and DF values had to be calculated according to the data available in the literature. For zinc sulphate, the EU Risk Assessment Report of Zinc Metal (JRC-IHCP, 2010) was used as data source; a molar conversion factor of 2.5 was applied to express the reported NOEC values in mg ZnSO$_4$/L. For acrylic acid, the disseminated REACH registration dossier was used as main data source (ECHA, 2011, 2016). For alachlor, the Aquatic impact indicators DAtabase (AiiDA, 2014) was used as main data source; AADIA provides test results gathered from reference databases such as the US EPA ECOTOX Database or the OPP Pesticide Ecotoxicity Database. The data collected from literature to calculate the CDV of zinc sulphate, acrylic acid and alachlor fulfilled the following criteria: data reliable without restriction (Klimisch 1) (Klimisch *et al*, 1997) or if not available, with restrictions (Klimisch 2); freshwater data (marine data were not

considered); toxicity data expressed as chronic NOEC or acute $E(L)C_{50}$ (chronic $E(L)C_{10}$ were not considered). The whole input data used to calculate the downstream impact scores by the CDV approach are presented in Table 4.3.

Table 4.3: Input data used to calculate by the CDV approach the downstream impact score of each ingoing substance identified in the virtual product*

Substance name	Acute $L(E)C_{50}$ (mg.L^{-1})	Chronic NOEC (mg.L^{-1})	SF	TF	DF	Data source
LAS	//	0.69	10	0.069	0.05	DID-list v2014.1 – Part A (Ingredient DID-no. 2001)
Acetic acid	30	//	1000	0.03	0.05	DID-list v2014.1 – Part A (Ingredient DID-no. 2567)
Ethanol	1000	//	1000	1	0.05	DID-list v2014.1 – Part A (Ingredient DID-no. 2529)
Zinc sulphate	//	0.087	10	0.0087	1	EU Risk Assessment Report of Zinc Metal (JRC, 2010)
BIT	//	0.04	10	0.004	0.5	DID-list v2014.1 – Part A (Ingredient DID-no. 2401)
Acrylic acid	//	0.129	50	0.0026	0.05	REACH disseminated dossier (ECHA, 2011; 2016)
Alachlor	//	0.1	10	0.01	1	Aquatic Impact Indicators DAtabase (AiiDA, 2014)

*It should be noted that in the scope of this work no cross-validation of the input data in the USEtox versus the DID-list database has been performed. We presently do not know what impact this had on the comparisons.

4.3   Results

4.3.1   Upstream impact scores

The individual impact scores calculated by the USEtox approach are presented in Table 4.4. Zinc sulphate, BIT and alachlor are the three substances showing the highest upstream impact scores with a calculated $CF_{upstream}$ of 83.5, 60.4 and 60.0 PAF.m^3.day.kg^{-1}, respectively. Lower impact scores are obtained with LAS, acetic acid, ethanol and acrylic acid, which all exhibit a $CF_{upstream}$ in the range 0.2-0.8 PAF.m^3.day.kg^{-1}. It is to note that an upstream impact score of 7.2E-04 PAF.m^3.day.kg^{-1}, although negligible, is obtained for water due to production/recycling expenses. Taking into account the relative contribution of each substance, an *upstream* impact score of 1.56 PAF.m^3.day.kg^{-1} is obtained for the whole virtual product, the major contributors being zinc sulphate (53.4%) and BIT (38.7%) (Table 4.5).

Table 4.4: Upstream impact scores calculated by the USEtox approach for each ingoing substance identified in the virtual product

Substance name	CF$_{upstream}$ – USEtox v1.01	
	PAF.m^3.day.kg^{-1} substance	Ranking
LAS	0.79	5
Acetic acid	0.80	4
Ethanol	0.26	7
Zinc sulphate	83.50	1
BIT	60.40	2
Acrylic acid	0.41	6
Alachlor	60.00	3
Water	<0.01	8

Note$_1$: numbers are reported as rounded values.

Note$_2$: water does have an upstream impact due to production/recycling expenses.

Table 4.5: Relative contribution of each ingoing substance to the upstream impact score calculated for the virtual product by the USEtox approach

Substance name	CF$_{upstream}$ – USEtox v1.01		
	PAF.m^3.day.kg^{-1} product	% CF$_{upstream}$ product	Ranking
LAS	0.04	2.53	4
Acetic acid	0.04	2.56	3
Ethanol	0.01	0.83	6
Zinc sulphate	0.84	53.44	1
BIT	0.60	38.65	2
Acrylic acid	<0.01	0.03	8
Alachlor	0.03	1.92	5
Water	<0.01	0.04	7
	TOTAL	TOTAL	
Virtual product	1.56	100	

Note: numbers are reported as rounded values.
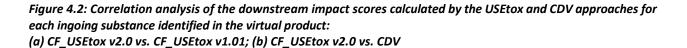
4.3.2   Downstream impact scores
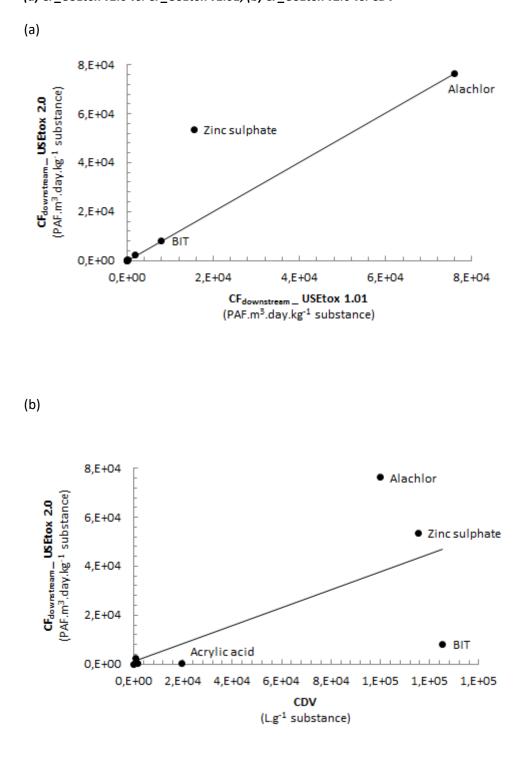
The absolute impact scores calculated by the USEtox and CDV approaches are presented in Table 4.6. The three substances having the highest downstream impact scores are zinc sulphate, BIT and alachlor, whatever the approach (USEtox or CDV) or the model (USEtox v1.01 or v2.0) used. As illustrated in Figure 4.2.a, the scores provided by USEtox v2.0 are almost identical to the one provided by USEtox v1.01, except for zinc sulphate: the $CF_{downstream}$ of zinc sulphate is indeed more than tripled when passing from v1.01 to v2.0 (ratio: 3.43). Excluding zinc sulphate from the dataset, a squared Pearson correlation coefficient R^2 of 1 is obtained; including zinc sulphate in the dataset, the correlation coefficient goes down to 0.79. When comparing the scores provided by USEtox v2.0 and by CDV calculation, a squared Pearson correlation coefficient R^2 of 0.47 is obtained; this poor correlation is illustrated in Figure 4.2.b.

Table 4.6: Downstream impact scores calculated by the USEtox and CDV approaches for each ingoing substance identified in the virtual product

Substance name	$CF_{downstream}$ – USEtox v1.01		$CF_{downstream}$ – USEtox v2.0		CDV	
	PAF.m^3.day.kg^{-1} substance	Ranking	PAF.m^3.day.kg^{-1} substance	Ranking	L.g^{-1} substance	Ranking
LAS	2000.0	4	2089.4	4	724.6	6
Acetic acid	50.0	6	50.0	6	1666.7	5
Ethanol	3.1	7	2.7	7	50.0	7
Zinc sulphate	15600.0	2	53591.9	2	115273.8	2
BIT	7910.3	3	7912.8	3	125000.0	1
Acrylic acid	200.0	5	200.5	5	19379.8	4
Alachlor	76000.0	1	76298.4	1	100000.0	3
Water	0.0	8	0.0	8	0.0	8

Note: numbers are reported as rounded values.

Figure 4.2: Correlation analysis of the downstream impact scores calculated by the USEtox and CDV approaches for each ingoing substance identified in the virtual product:
(a) CF_USEtox v2.0 vs. CF_USEtox v1.01; (b) CF_USEtox v2.0 vs. CDV

(a)

(b)

Taking into account the contribution of each substance, a *downstream* impact score of 376.0 and 760.5 PAF.m^3.day.kg^{-1} is obtained for the whole virtual product with USEtox v1.01 and v2.0, respectively; in both cases, the major contributor is zinc sulphate (41.5 and 70.5%, respectively) followed by LAS (26.6 and 13.7%, respectively) and BIT (21.0 and 10.4%, respectively). By the CDV approach, a downstream impact score of
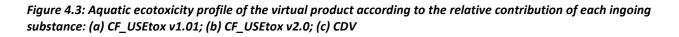
2594.18 L.g^{-1} is obtained for the whole virtual product, the major contributors being BIT (48.2%) and zinc sulphate (44.4%) (Table 4.7).
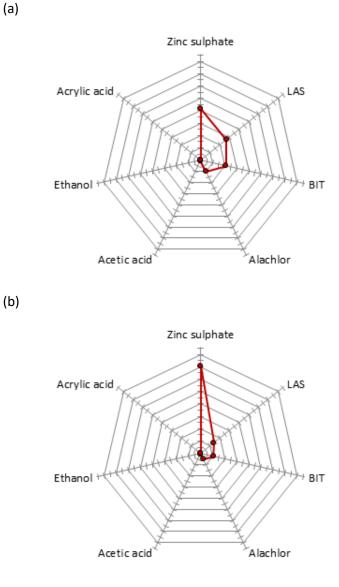
The relative contribution of each substance to the whole 'profile' of the virtual product is further illustrated in Figure 4.3 which clearly differentiates the USEtox approach (profile driven by the toxicity of zinc sulphate – especially with USEtox 2.0) and the CDV approach (profile balanced by the toxicity of zinc sulphate and BIT).

Table 4.7: Relative contribution of each ingoing substance to the downstream impact score calculated for the virtual product by the USEtox and CDV approaches

Substance name	CF$_{downstream}$ – USEtox v1.01			CF$_{downstream}$ – USEtox v2.0			CDV		
	PAF.m^3.day.kg^{-1} product	% CF$_{downstr.}$ product	Ranking	PAF.m^3.day.kg^{-1} product	% CF$_{downstr.}$ product	Ranking	L.g^{-1} product	% CDV product	Ranking
LAS	**100.0**	26.60	2	**104.5**	13.74	2	**36.23**	1.40	5
Acetic acid	**2.5**	0.66	5	**2.5**	0.33	5	**83.33**	3.21	3
Ethanol	**0.2**	0.04	7	**0.1**	0.02	7	**2.50**	0.10	7
Zinc sulphate	**156.0**	41.49	1	**535.9**	70.47	1	**1152.74**	44.44	2
BIT	**79.1**	21.04	3	**79.1**	10.40	3	**1250.00**	48.18	1
Acrylic acid	**0.2**	0.05	6	**0.2**	0.02	6	**19.38**	0.75	6
Alachlor	**38.0**	10.11	4	**38.2**	5.02	4	**50.00**	1.93	4
Water	**0.0**	0.00	8	**0.0**	0.00	8	**0.00**	0.00	8
	TOTAL	TOTAL		TOTAL	TOTAL		TOTAL	TOTAL	
Virtual product	**376.0**	100.00		**760.5**	100.00		**2594.18**	100.00	

Note: numbers are reported as rounded values.

Figure 4.3: Aquatic ecotoxicity profile of the virtual product according to the relative contribution of each ingoing substance: (a) CF_USEtox v1.01; (b) CF_USEtox v2.0; (c) CDV

(a)

(b)

(c)

4.3.3 Downstream versus upstream impact scores

The upstream, downstream and total impact scores calculated with USEtox v1.01 are presented in Table 4.9. Considering the whole life cycle of the virtual product, the upstream stage (= 'Raw materials') only represent 0.4% of the total estimated impact on the environment. At the opposite, the downstream stage (= 'Disposal') represent 99.6% of the total estimated impact.

Table 4.9: Relative contribution of each ingoing substance to the upstream, downstream and total impact scores calculated for the virtual product by the USEtox approach

Substance name	$CF_{upstream}$ – USEtox v1.01		$CF_{downstream}$ – USEtox v1.01		CF_{total} – USEtox v1.01	
	$PAF.m^3.day.kg^{-1}$ product	% CF_{total} product	$PAF.m^3.day.kg^{-1}$ product	% CF_{total} product	$PAF.m^3.day.kg^{-1}$ product	% CF_{total} product
LAS	**0.04**	0.01	**100.0**	26.60	**100.0**	26.5
Acetic acid	**0.04**	0.01	**2.50**	0.66	**2.5**	0.67
Ethanol	**0.01**	<0.01	**0.2**	0.04	**0.2**	0.05
Zinc sulphate	**0.84**	0.14	**156.0**	41.49	**156.8**	41.54
BIT	**0.60**	0.10	**79.1**	21.04	**79.7**	21.11
Acrylic acid	**<0.01**	<0.01	**0.2**	0.05	**0.2**	0.05
Alachlor	**0.03**	<0.01	**38.0**	10.11	**38.0**	10.07
Water	**<0.01**	<0.01	**0.0**	0.00	**0.00**	<0.01
	TOTAL	TOTAL	TOTAL	TOTAL	TOTAL	TOTAL
Virtual product	**1.6**	0.4	**376.0**	99.6	**377.5**	100.00

Note: numbers are reported as rounded values.

5. DETAILED ANALYSIS OF CASE STUDY RESULTS

The purpose of this chapter is to enhance the insight in the final figures of the case study and elucidate general principles in both life cycle stages leading up to the result.

5.1 Upstream Impacts (Aquatic Ecotoxicity)

Databases are used in nearly every LCA study to cover all those steps for which the assessor cannot generate an explicit description in terms of material inputs and outputs. The system components which can typically be described well are all steps directly within the reach of the assessor. Within our case study this would mean the knowledge of the formulation in terms of input weights or the energy required to produce the virtual product, e.g. by a mixing of components. The explicit knowledge very often ends at the factory gates, however. While the weight percentages in the formulation might be considered to be known parameters to the LCA practitioner, the production of each component usually lies outside of ones' own factory gates. The same thinking applies to the pre-products required to manufacture each component still further upstream and so forth. A similar thinking shows that while demand for electrical energy can be tabulated, the impacts associated with energy production would be outside of one's own reach and inaccessible to ad hoc estimation. In order to get an estimation for impacts associated with the inaccessible system parts, such gaps in the assessment that exist in nearly every such study are typically filled with database datasets. An alternative is the use of supplier data, but due to the complexity of the real world these are likely to build on estimations and databases, too.

The perspective adopted by the LCA practitioner, e.g. as a producer of formulations, might not be the main contribution for any given assessment in an impact category. Major impacts can be incurred outside of one's own production facilities, e.g. by raw materials purchased and these are often filled in with database datasets. Due to its commonplace use it is thus necessary to identify the role databases play in the current scope of impact assessment of freshwater ecotoxicity.

In this following section we summarise the analysis of upstream impacts of database datasets used to cover upstream production steps and associated emissions. To this end we use the example of linear alkylbenzene sulphonate (LAS) and Zinc sulphate ($ZnSO_4$) as examples in our discussion. The origin of upstream toxicity is quite different for both substances, making this choice instructive to demonstrate the role that LCA databases play.

5.1.1 Dataset analysis: LAS

LAS is a dataset retrievable from Ecoinvent 2.2 Newer data for detergent components was produced in a current project of ERASM, but unavailable in the scope of this study. Also this is considered not to change the general learnings that can be extracted from the following analysis.

According to the documentation provided by Ecoinvent (Zah and Hischier, 2007), LAS is produced in a two-step process. The first step is the alkylation of benzene using $AlCl_3$ or HF. In the $AlCl_3$ process the benzene is

alkylated with chloro-paraffins and/or n-olefins with the help of an $AlCl_3$ catalyst. In the HF process, benzene is alkylated directly with n-olefins using HF as a catalyst. The n-olefins themselves are produced by catalytic dehydrogenation of n-paraffin's. In both processes the n-paraffins are responsible for the linearity of the alkyl chain (Zah and Hischier, 2007).

The second step is the sulphonation of alkyl benzenes with sulphuric acid or sulphur trioxide (SO_3). Finally, caustic soda is used to neutralise the acid that has been produces (Berna et al, 1995). About 30% of the LAS produced in Europe is manufactured via the aluminium chloride route ($AlCl_3$) and about 70% is produced via hydrofluoric acid (HF) (WHO, 1996).

The following Table 5.1 shows the inputs needed for LAS production.

Table 5.1: Unit process LCI with materials and processes needed for the production of LAS (functional unit is mass). Paraffin is the dominating input material in terms of mass.

Inputs		Unit
Chemicals		
HF	0.01	Kg
Al	0.01	Kg
Benzene	0.251	Kg
NaOH (50%)	0.127	Kg
Paraffin	0.516	Kg
Sulphur	0.1	Kg
Other Services / Infrastructure		
Chemical plant	4E-10	pieces
Transport rail	0.6	tkm
Transport truck	0.1	tkm

Dominant contributions to the impact score of LAS stem from emissions coming from paraffin (28%), aluminium production (20%), Chemical plant – organics (15%) and Caustic Soda (12%). Here Chemical plant – organics is an infrastructure related impact, which captures the emissions due to the provision of required production facilities.

Overall, these datasets are the level 1 datasets (please refer chapter 2 for an explanation of the meaning of these LCA dataset specifics, in particular to Figure 2.1), constituting the unit process of LAS production. While a first analysis of the data shows which of the constituents of the unit process shown in Table 5.1 have which share in the overall impact, it is not clear at this stage as to which environmental emissions cause the impact-score.

Using the aggregated dataset for the LAS production gives an answer to this question. This aggregated dataset differs from the unit process dataset of LAS shown in Table 5.1 in so far, as only environmental flows are listed therein and these can be directly submitted to LCIA, i.e. scored using the CFs of USEtox (please refer to chapter

2.4 for further explanation of LCIA). The flows in Table 5.1 are all intermediate flows and these cannot be scored directly. Figure 5.1 shows the contributions to the impact score in percent. The impact is seen to be caused by heavy metals, most of all chromium emitted to waterbodies, which might seem counterintuitive to those not familiar with LCA. As explained in chapter 2.4, however, LCA databases are complex constructs, in which datasets can be interpreted to be forming large trees based on connections made by the intermediate flows. The primary flows or environmental emissions can be defined to happen within all unit processes interconnected. Thus, the unit process for LAS shown in Table 5.1 is only the beginning of a large tree structure, where emissions happen along its traversal. The emissions in the production of LAS are clearly seen not to happen at the topmost level. So while it can be stated from the aggregate dataset of LAS that Chromium is the leading environmental impact, it is not clear at which levels of the hierarchy these emissions happen and thus it is not possible to state offhand which processes along the upstream value chain of LAS cause the impact.

An analytic approach would have to be used to unravel the dataset hierarchy to gain further insight into which datasets beyond level 1 cause the chromium emissions making such a large contribution to the impact.

The hierarchy beyond level 1 shows that at deeper levels identification of commonalities is possible and aggregation on the basis of a common dataset or by a type of process or service is certainly helpful. Approaching the hierarchy up to level 5 for LAS we identified electrical energy to be one recurring theme, making approx. 100 appearances in other unit processes and contributing an aggregated 13% to the impact score through the dataset 'electricity, medium voltage, production UCTE, at grid', which models an average European energy production. Going to deeper levels would add to the percentage, but it is not clear to which overall contribution it would converge.

Another strategy would be to follow the leading impact causing processes from level 1 downwards. In the case of LAS paraffin is the main impactor (28% of impact). Following the hierarchy of paraffin shows generation of energy by industrial furnaces to be the leading impact ('heat, heavy fuel oil, at an industrial furnace 1MW'). The impact is not related to combustion of the fuel itself in the production of paraffin, but rather tied to the provisioning of the fuel by a refinery as well as the storage of oil. Since we stopped with our analysis at this point in the value chain our conclusions must not be final. For example, it might be reasonable to assume that the provisioning of fuel is tied to infrastructure impacts, which are caused by the construction of the refinery out of metal parts and concrete, thus a possible explanation for the large share of impact by heavy metals in Figure 5.1. But it might as well be caused be the extraction of crude oil still some steps upstream and / or the infrastructure related to the crude oil extraction machinery.

The latter example shows that it is very tedious to follow the value chain upstream. Thus this is not very often done, although it can yield valuable insights and can help identify weaknesses in datasets. In the following we take a closer look at the production of electricity, which we identified to be one of the processes leading to emissions of chromium.
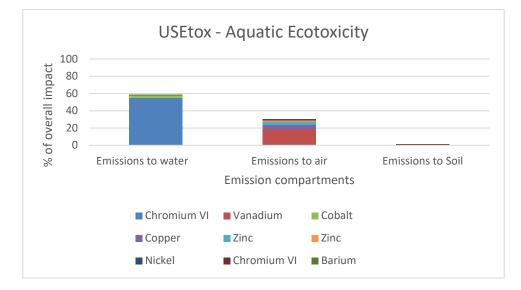
Electricity

The main impacts are caused by the pre-chains of the dataset 'electricity, medium voltage, production UCTE, at grid'. We located the main contributing unit processes and the most dominant primary flows in the pre-chains causing the toxic impacts by digging deeper into the hierarchy of datasets for electricity.

Medium voltage electricity is produced from electricity at high voltage by transformation from 'electricity, high voltage, production UCTE, at grid'. The latter dataset refers to 'electricity, production mix UCTE', which specifies the contributions of the individual countries participating in the continental European electricity grid. Here, Germany contributes roughly one quarter of the energy and has the highest share in the ecotoxicity score.

The highest contribution to ecotoxicity in the German electricity mix comes from 'electricity, lignite, at power plant'. Emissions related to disposal of wastes from lignite mining cause the overwhelming share of impact, dominated by spillages of chromium VI into groundwater.

Looking into the dataset 'disposal, spoil from lignite mining, in surface landfill', we find that a large number of output flows modelling leakages into groundwater have no characterisation factors assigned. This leads to uncertainty about the total impact value as described in section 'Life Cycle Impact Assessment' in chapter 2.4.3 'Reliability and Accuracy in LCIA' above, where we describe case 1) as the case where elements CF_i are undefined in the LCIA, thus effectively assigning the associated flows a contribution of 0.0. This is something that becomes visible only during a deeper analysis of the data and would not be transparent during a standard LCA. Among the substances exceeding the emissions of cobalt in size and which are not assigned a characterisation factor in Ecoinvent are 'nickel, ion', 'zinc, ion', strontium, aluminium, sulphate and phosphate. Their omission from the total impact value leads to an underestimation of the impact.

Figure 5.1: Upstream impacts of LAS by substance as calculated with Ecoinvent2.2, displayed for the major contributors, in percent. The impact mainly consists of emissions to water (59%) and emissions to air (31%). The multimedia fate modelling underlying USEtox makes emissions to air contribute to aquatic ecotoxicity. Chromium VI, Vanadium & Copper account for 79% of the impact.

5.1.2   ZnSO4

In Ecoinvent 2.2 zinc sulphate is modelled as being produced by treatment of zinc oxide with sulphuric acid (Hischier et al, 2007). The authors cite Ullmann's Encyclopedia of Industrial Chemistry (Rohe and Wolf, 2007) in its seventh edition as the main source for their modelling. According to information in the dataset
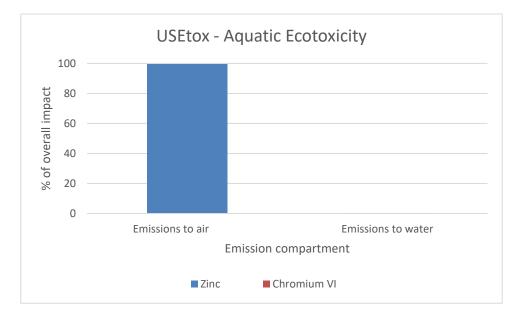
description, several inputs had to be estimated with proxy data as the main source could not provide any information. For example, a different process was used as a proxy to fill the energy requirements for the drying process (quicklime kiln process). Emissions to air and water compartments were estimated due to absence of primary information.

The result of the contributions of emissions to the different environmental compartments in percent is displayed in Figure 5.2.

Table 5.2: Unit process LCI with materials and processes needed for the production of 1 kg ZnSO4

Input material		Unit
Chemicals		
Sulphuric acid	0.575	kg
Zinc oxide	0.478	kg
Other Services / Infrastructure		
Chemical plant	4E-10	pieces
Thermal energy	3.742	MJ
Transport rail	0.6318	tkm
Transport truck	0.1053	tkm

Figure 5.2: Upstream impacts of ZnSO4 by substance as calculated with Ecoinvent2.2, displayed for the major contributors, in percent. The impact mainly consists of zinc emissions to air (99.5%), stemming from the final step in the manufacturing process of ZnSO4. The multimedia fate modelling underlying USEtox makes emissions to air contribute to aquatic ecotoxicity. Direct emissions to water play a negligible role (Chromium VI at 0.3% of the overall impact).

5.1.3   Conclusions Upstream Impacts

LCA covers impacts along all life cycle stages included in the scope of a study. Since we used aggregated datasets of raw materials from an LCA database, Ecoinvent, we include all stages in the production of chemicals and supplementary materials and services (e.g. energy, transport, and infrastructure) up to extraction of the most basic raw materials from the biosphere. This procedure is perfectly acceptable in LCA and at the heart of life cycle thinking.

Both exemplarily analysed raw materials exhibit different lead contributions to the freshwater ecotoxicity. For LAS long term emissions of heavy metals several levels upstream play a dominant role in the overall impact. This poses a striking difference to RA, where supplementary materials and services are not linked into the assessment. For $ZnSO_4$ the main impact stems from the final production step and is associated with air emissions of zinc, thus being more closely related to the thinking exerted in RA. USEtox implicitly calculates the fate of the substance in the environment and scores the impact resulting from exposure in freshwater bodies.

The exemplary analysis shows, that in principle it is possible to follow and analyse the individual impacts of each data set and its predecessors. In practice, however, this is rarely done due to the time requirements associated with it.

The overall ecotoxicological impact of the upstream contribution is small compared to the disposal stage situated downstream in the case study. This may hold true for all products disposed of with in wastewater, but should not be generalised. Depending on the mode of use / disposal and the risk management measures in place the relation could shift towards the upstream impact. Since USEtox implicitly considers the environmental fate of substances, even emissions to e.g. air are linked to freshwater ecotoxicity through environmental multi-compartment distribution.

5.2   Downstream Contributions

5.2.1   Comparison of results of USEtox and CDV

From the case study described in Chapter 4, a rough analysis of the results shows that the major contributions to the overall downstream impact score of the virtual product come from zinc sulphate (USEtox: 41.5-70.5%; CDV: 44.5%), BIT (USEtox: 10.4-21%; CDV: 48.2%) and LAS (USEtox: 13.7-26.6%). A deeper look to the results however demonstrates great divergences from one model to another, as evidenced for example by the poor correlation observed between the relative and absolute scores provided by the USEtox and CDV methods. This could be somewhat surprising at a first glance as both methods are based on comparable aquatic fate and ecotoxicity data. It can thus be wondered whether the divergences observed are related to mechanisms inherent to the models or to external independent factors.

In fact, differences in results obtained with USEtox and CDV are based on differences in the models, but are also due to the data used in the parametrization of either model. The data can furthermore be different

regarding A) the data sources being used and B) the endpoints towards which the data were interpreted or both.

An example for A) would be the (systematic or coincidental) use of a different database or datasets measured for different species and an example for B) the use of chronic data versus acute data or a different transformation of the data basis in derivation of assessment factors such as the EC_{50}.

Both factors A) and B) complicate the quantitative comparison of results generated with either model, as a significant share of differences in the assessment may be rooted in a choice of basic parameters. Insofar as they are A) coincidental, these differences should not be attributed to the models characteristics, while a prescribed selection of parameters in A) and use of different endpoints in B) can be attributed to model differences.

It would be instructive to carry out such a detailed analysis and eventually reparametrize the models for the virtual formulation using the same data sources wherever possible to minimise differences arising due to A). While such a project would be expected to yield valuable insights it is beyond the scope of the present ECETOC task force.
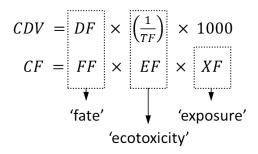
In order to still gain an insight into the reasons for the differences in results obtained with CDV and USEtox it is instructive to analyse the fate and exposure modelling of the analysis determined by the parameters adopted in the case study.

5.2.2   USEtox v2.0 versus USEtox v1.01

For the case study, USEtox impact factors were calculated using two versions of the model: v1.01 and v2.0. Both versions of the model provided very similar results for most of the substances except zinc sulphate: the CF of the latter is indeed more than tripled between USEtox v1.01 and v2.0. This major evolution is obviously related to an update of the databases linked to the model between 2010 (release date of USEtox v1.01) and August 2015 (release date of USEtox v2.0). As evidenced from Table 4.2b (*cf.* Chapter 4), there was a major update of the $avlogEC_{50 \, zinc \, sulphate}$ (from 0.02 to -0.75 mg.L^{-1} – log transformed) in USEtox v2.0 – Database Organics; thus new (and more severe) ecotoxicity data were obviously included in the most recent version of the database. Of note, zinc sulphate is the only substance from the study case for which the $avlogEC_{50}$ value changed between USEtox v1.01 and v2.0. For other substances, updates concerned other input parameters (*e.g.* Koc, BAF_{fish}) but it is interesting to note that those changes had very little influence on the calculated impact scores.

5.2.3   USEtox (v2.0) versus CDV

Although CF (USEtox) and CDV are not expressed in the same unit, they both integrate parameters characterising the freshwater fate and ecotoxicity of the substance considered:

$$CDV = \boxed{DF} \times \boxed{\left(\frac{1}{TF}\right)} \times 1000$$

$$CF = \boxed{FF} \times \boxed{EF} \times \boxed{XF}$$

'fate'   'exposure'

'ecotoxicity'

Besides, unlike CDV, CF integrates an additional exposure parameter referring to the fraction of the substance dissolved in freshwater. The whole fate, ecotoxicity and exposure parameters obtained from the study case are detailed in Table 5.3.a and 5.3.b.

Table 5.3: Values of (a) USEtox parameters and (b) CDV parameters obtained from the case study

(a)

Substance name	EF [PAF.kg^{-1}.m^3]	FF [d]	XF [-]	CF [PAF.m^3.day.kg^{-1}]
LAS	1.11E+02	1.88E+01	1.0	2.09E+03
Acetic acid	4.35E+00	1.15E+01	1.0	5.00E+01
Ethanol	3.35E-01	8.05E+00	1.0	2.69E+00
Zinc	*2.84E+03*	*9.41E+01*	*0.5*	*1.34E+05*
Zinc sulphate	//	//	//	0.54E+05*
BIT	4.21E+02	1.88E+01	1.0	7.91E+03
Acrylic acid	1.75E+01	1.15E+01	1.0	2.01E+02
Alachlor	1.42E+03	5.36E+01	1.0	7.63E+04

* As the Database Inorganics (USEtox v2.0) contains data for metals but not for metal salts, the CF for zinc sulphate was deduced from the one of zinc metal using a molar conversion factor of 0.4 (= 1/[M$_{zinc\ sulphate}$/M$_{zinc}$]). The fate of zinc sulphate was assumed to be parametrized in USEtox the same way as zinc metal.

(b)

Substance name	TF [mg.L^{-1}]	1/TF [L.mg^{-1}]	DF [-]	CDV [L.g^{-1}]
LAS	6.90E-02	1.45E+01	0.05	7.25E+02
Acetic acid	3.00E-02	3.33E+01	0.05	1.67E+03
Ethanol	1.00E+00	1.00E+00	0.05	5.00E+01
Zinc sulphate	8.75E-03	1.15E+02	1.00	1.15E+05
BIT	4.00E-03	2.50E+02	0.50	1.25E+05
Acrylic acid	2.58E-03	3.88E+02	0.05	1.94E+04
Alachlor	1.00E-02	1.00E+02	1.00	1.00E+05

Although the calculation of CF in USEtox integrates an exposure parameter (XF) not considered in the calculation of CDV, this parameter does not solely explain the divergences observed between CF and CDV impact scores. As evidenced in Table 5.3.a, a XF value of 1 was attributed to every substance in the virtual product, except for zinc (XF = 0.5). As reported in the USEtox™ User Manual v1.01 (Huijbregts *et al*, 2010): *"the environmental exposure factor is calculated by:*

$$FR_{w.w} = \frac{1}{1 + (Kp \cdot SUSP + K_{doc} \cdot DOC + BCF_{fish} \cdot BIOmass)/1 \cdot 10^6}$$

where Kp is the partition coefficient between water and suspended solids (l/kg), SUSP the suspended matter concentration in freshwater (= 15 mg/l in USEtox™), K_{doc} the partitioning coefficient between dissolved organic carbon and water, DOC the dissolved organic carbon concentration in freshwater (= 5 mg/l in USEtox™), BCF_{fish} the bioconcentration factor in fish (l/kg) and BIOmass the concentration of biota in water (= 1 mg/l in USEtox™)."

Zinc was thus the only one substance for which the USEtox model assumed a partial adsorption to organic carbon in the freshwater compartment. By the way, as USEtox dataset does not contain data on metal salts, the CF of zinc sulphate had to be deduced from the one of zinc metal; this implies that the exposure parameter (and to a higher extent, the fate parameter) provided by USEtox for zinc metal had 'by default' to be applied to zinc sulphate although one can expect both entities to behave somewhat differently in the environment. This raises some questions about the possibility to get relevant impact scores for metal salts from USEtox. Anyway, as the exposure parameter can be laid aside in the comparative analysis of CF and CDV, the ecotoxicity and fate parameters appear as the ones which drive to a large extent the impact scores obtained in the study case.

In the CDV approach, the fate parameter (DF) is very simplistic as it only reflects the biodegradation behaviour of a substance in water. In the USEtox approach, the fate parameter (FF) is more complex as it integrates the degradation and partitioning behaviour of the substance between the different environmental compartments. The fate parameter can thus explain part or all of the divergences observed between the USEtox and CDV approaches. To test this hypothesis, the following exercise was performed: for each substance in the virtual product, the USEtox v2.0 input data were used to calculate an impact score according to the CDV approach; the scores thus obtained (CDV_{USEtox}) were then compared to the ones initially calculated with USEtox (CF). For the aim of the exercise, DF_{USEtox} and TF_{USEtox} had first to be calculated for every substance.

In USEtox databases, information related to the biodegradability of substances in water is available in the form of a degradation constant $K_{deg\,W} = \ln(2)/DT50$, expressed in s^{-1}. For each substance in the virtual product, this constant was used to calculate the half-lives (d) in water. The DT50 values thus obtained were then converted into one of the biodegradation category used for DF calculation, i.e. 'Readily biodegradable', 'Readily biodegradable, failing 10-day window', 'Inherently biodegradable', or 'Not biodegradable/Persistent'. The conversion was made in accordance with the threshold values reported in Table 5.4. In the end, the DF_{USEtox} values were determined according to the data reported in Table 4.3 (cf. Chapter 4); the DF_{USEtox} values obtained this way are reported in Table 5.5.

Table 5.4: First order rate constants and half-lives for biodegradation in surface water estimated based on results of screening tests on biodegradability (adapted from OECD, 2004)

Study result	Rate constant $(K_{deg\,W})$ [d^{-1}]	Water half-life [d]
Ready biodegradable	0.047	15
Ready biodegradable, failing 10-day window	0.014	50
Inherently biodegradable	0.0047	150
Not biodegradable/Persistent	0 (6.93E-7 EUSES-default)	To be determined (1000000 EUSES-default)

Table 5.5: DF$_{USEtox}$ determined from USEtox v2.0 dataset (Database Organics, Database Inorganics)

Substance name	Kdeg W [s-1]	Half-life [d]	DFUSEtox [d]
LAS	5.35E-07	15.0	0.05
Acetic acid	9.25E-07	8.7	0.05
Ethanol	9.25E-07	8.7	0.05
Zinc sulphate	1.00E-20	8.02E14	1.00
BIT	5.35E-07	15.0	0.05
Acrylic acid	9.25E-07	8.7	0.05
Alachlor	1.34E-07	59.9	0.15

For LAS, acetic acid, ethanol, BIT and acrylic acid, the half-lives deduced from the $K_{deg\,W}$ values were in the range 8.7-15 days, which was interpreted as *'Readily biodegradable'* (DF = 0.05); for alachlor, the half-life was slightly higher than 50 days, which was interpreted as *'Readily biodegradable, failing 10-d window'* (DF = 0.15); for zinc sulphate, the half-life was very high and was thus interpreted as *'Persistent'* (DF = 1). It is interesting to note here that the DF obtained this way from the USEtox dataset were identical to the one obtained from the CDV input dataset, except for BIT (DF$_{CDV}$ = 0.5) and alachlor (DF$_{CDV}$ = 1). This highlights the influence of the data source when comparing two methods with different datasets.

In USEtox databases, information related to the toxicity of substances towards aquatic species is available in the form of a log-transformed Hazardous Concentration for 50% of species (log HC$_{50}$), also called avlogEC$_{50}$ and expressed in mg.L^{-1}. For each substance in the virtual product, the average chronic EC$_{50}$ (geometric mean) was determined from the HC$_{50}$ value (anti-log transformation). The chronic EC$_{50}$ value thus obtained was then converted into a chronic NOEC value using the following extrapolation factor: Chronic EC$_{50}$/Chronic NOEC = *ca.* 5 (Payet, 2004). A SF of 10 was then applied to calculate the TF$_{USEtox}$ value, assuming that the standards trophic levels (*i.e.* fish, aquatic invertebrates, algae) were all represented in the chronic NOEC; the TF$_{USEtox}$ values calculated this way are reported in Table 5.6.

Table 5.6: TF$_{USEtox}$ determined from USEtox v2.0 dataset (Database Organics, Database Inorganics)

Substance name	HC50 [mg.L^{-1}]	Chronic EC^{50} [mg.L^{-1}]	Chronic NOEC [mg.L^{-1}]	TF$_{USEtox}$ [mg.L^{-1}]
LAS	0.65	4.47	0.89	0.089
Acetic acid	2.06	114.82	22.96	2.296
Ethanol	3.17	1479.11	295.82	29.582
Zinc	*-0.75*	*0.18*	*//*	*//*
Zinc sulphate	//	0.44*	0.09	0.009
BIT	0.07	1.17	0.23	0.023
Acrylic acid	1.46	28.84	5.77	0.577
Alachlor	-0.45	0.35	0.07	0.007

*As the Database Inorganics (USEtox v2.0) contains data for metal elements but not for metal salts, the chronic EC$_{50}$ for zinc sulphate was deduced from the one of zinc element using a molar conversion factor of 2.5 (= Mzinc sulphate/Mzinc).

The DF$_{USEtox}$ and TF$_{USEtox}$ values calculated from the USEtox v2.0 input dataset were eventually used to calculate for each substance an absolute impact score (corresponding to 100% of the substance) and a relative impact score (taking into account the %-content of the substance in the virtual product) according to the CDV approach; the CDV$_{USEtox}$ values calculated this way are reported in Table 5.7. For comparative purpose, the CF values originally calculated from the USEtox v2.0 dataset are reminded in Table 5.8.

Table 5.7: CDV$_{USEtox}$ determined from USEtox v2.0 dataset (Database Organics, Database Inorganics)

Substance name	Absolute CDV [L.g^{-1}]	Ranking	Relative CDV [L.g^{-1}]	Relative CDV (% CDV$_{product}$)	Ranking
LAS	559.68	4	27.98	2.36	2
Acetic acid	21.77	6	1.09	0.09	5
Ethanol	1.69	7	0.08	0.01	7
Zinc sulphate	112468.27	1	1124.68	94.85	1
BIT	2127.85	3	21.28	1.79	3
Acrylic acid	86.68	5	0.09	0.01	6
Alachlor	21137.87	2	10.57	0.89	4
Virtual product			1061,53	100	

Table 5.8: CF$_{USEtox}$ determined from USEtox v2.0 dataset (Database Organics, Database Inorganics)

Substance name	Absolute CF [PAF.m³.day.kg⁻¹]	Ranking	Relative CF [PAF.m³.day.kg⁻¹]	Relative CF (% CF$_{product}$)	Ranking
LAS	2089.42	4	104.47	13.74	2
Acetic acid	49.95	6	2.50	0.33	5
Ethanol	2.69	7	0.13	0.02	7
Zinc sulphate	53591.95	2	535.9	70.47	1
BIT	7912.80	3	79.13	10.4	3
Acrylic acid	200.52	5	0.20	0.02	6
Alachlor	76298.44	1	38.15	5.02	4
Virtual product			760.50	100	

When comparing the absolute scores obtained from USEtox v2.0 and CDV calculation, a squared Pearson correlation coefficient R^2 of 0.39 is obtained. If the CF of zinc sulphate is adjusted to assume 100% dissolution in freshwater (*i.e.* using XF = 1 instead of 0.5), the correlation coefficient rises to 0.78. If zinc sulphate is excluded from the analysis, a perfect correlation of the results is obtained (R^2 = 1). From above analysis, the following conclusions can be raised:

- for substances with no specific partitioning behaviour (*e.g.* LAS, acetic acid, ethanol, BIT, acrylic acid, alachlor), the USEtox and CDV approaches lead to comparable impact scores, provided that the input dataset is the same;

- having the biodegradability characterised by a continuous variable (USEtox: FF, in days) or a discrete variable (CDV: DF = 0.01, 0.05, 0.15, 0.5 or 1) has no influence on the impact scores;

- for substances with a specific partitioning behaviour (*e.g* zinc), the USEtox and CDV approaches provide different impact scores, even with an identical input dataset. As partitioning coefficients are not taken into account in the CDV calculation, the latter actually tends to maximise the residence time/fraction of substances in water. At the opposite, the CF calculation tends to be more realistic as partitioning coefficients are taken into account both in the exposure parameter (XF) but also the fate parameter (FF). Indeed, applying a XF of 1 instead of 0.5 to adjust the CF of zinc sulphate improved the correlation between the impact scores but a perfect correlation was not obtained. This clearly shows that in USEtox the fate parameter is not influenced only by the biodegradation potential of the substances.

Going further in the analysis, a closer look was given to the ranges of the fate and ecotoxicity parameters used in the study case; the corresponding orders of magnitude were calculated and are reported in Table 5.9.a and 5.9.b.

Table 5.9: Ranges of (a) USEtox parameters and (b) CDV parameters used in the case study

(a)

Substance name	Higher value	Lower value	Ratio	Order of magnitude
CF	1.34E+05	2.69E+00	4.97E+04	4
EF	2.84E+03	3.35E-01	8.47E+03	3
FF	9.41E+01	8.05E+00	1.17E+01	1
XF	1.00E+00	5.00E-01	2.00E+00	0
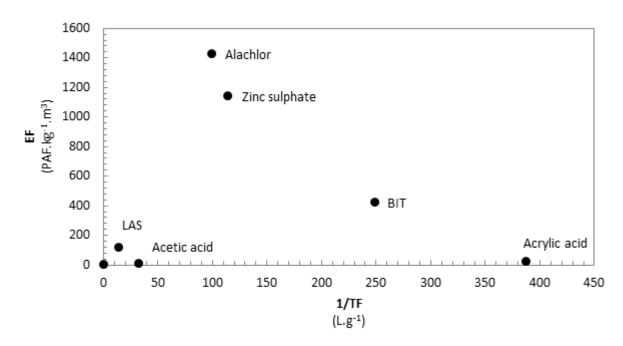
(b)

Substance name	Higher value	Lower value	Ratio	Order of magnitude
CDV	1.15E+05	5.00E+01	2.30E+03	3
1/TF	3.88E+02	1.00E+00	3.88E+02	2
DF	1.00E+00	5.00E-02	2.00E+01	1

In both the USEtox and CDV approaches, the ecotoxicity parameter covers a much wider range than the fate parameter. Thus, in both approaches, the ecotoxicity parameter is theoretically the one having the most influence on the final impact score.

As shown in Figure 5.3, the ecotoxicity parameter applied for CF calculation (EF) and the one applied for CDV calculation (1/TF) do not evolve the same way.

Figure 5.3: Comparison of the ecotoxicity parameters applied for CF calculation (EF) and CDV calculation (1/TF)

A first possible explanation to the divergence observed between EF and 1/TF lies to the fact that the USEtox-CF and CDV approaches do not use ecotoxicity data in the same way. For CF calculation, the ecotoxicity parameter is established from a geometric average of available data whereas for CDV calculation, this parameter is established from the data obtained on the most sensitive trophic level between algae, crustaceans and fish. In detail:

- ❖ The idea underlying the calculation of CF, *i.e.* considering an average, is to get a representative overview of the potentially affected fraction of species (PAF): CF integrates indeed species sensitivity distributions (SSD) and is calculated on the basis of a concentration (HC_{50}) ensuring the protection of 50% of the species. Besides, using an average avoids discriminating substances for which numerous data exist in regards of substances for which few data are available: the larger the set of data, the higher the probability of introducing a very sensitive species in the analysis.
- ❖ The idea underlying the calculation of CDV, *i.e.* considering only the most sensitive trophic level, is to ensure the protection of the maximum number of species.

In a study from Martz *et al* (2015), the environmental impact factors of 244 cosmetic substances and 577 shampoo formulae were calculated for the disposal stage according to the CDV method, the USEtox method and a modified version of the USEtox method (mod-USEtox). In the mod-USEtox method, the ecotoxicity parameter TF calculated with the CDV method was incorporated in the USEtox model, instead of the usual EF parameter. The underlying idea was to take into account the most sensitive aquatic species in the USEtox-CF calculation. Doing this way, Martz *et al* (2015) noticed a better correlation between the CF and CDV impact scores when using the mod-USEtox method in comparison to the original USEtox method. The correlation was however lower for formulae than for substances. Thus, even though CDV and USEtox-CF can be well correlated at the substance level, the weighing (% w/w) of substances in the formulae can strongly modify the impact scores obtained at the formula level.

Another possible explanation to the divergence observed between EF and 1/TF lies in the fact that USEtox-CF and CDV approaches integrate different levels of uncertainty when processing available ecotoxicity data to derive an ecotoxicity parameter. In USEtox for example, extrapolation factors are usually applied to derive the EF parameter: *"In USEtox, we calculate aquatic ecotoxicological effect factors based on geometric means of single species EC_{50} tests data. Chronic values have priority as long as they represent measured EC_{50} values. Note that chronic EC_{50} values (which would not require extrapolation) are rarely reported. Second-order priority is given to acute data, applying an acute-to-chronic extrapolation factor that is set to a default factor of 2 […] for organic substances […] and to a factor of 10 (crustaceans) and 20 (fish) and their average of 15 (all other trophic levels) for inorganic substances (cationic metals) […]"* (Huijbregts *et al*, 2015b). For CDV calculation, a SF in the range 10-10000 is applied according to the type of data available (acute or chronic) and to the number of trophic levels assessed (one, two or three among: fish, aquatic invertebrates and algae).

In the end, it appears difficult at this moment to precisely explain the divergence observed between the USEtox-CF and CDV impact scores in our case study, and also in the published case studies. This is all the more difficult as the databases linked to USEtox and the ones used for CDV calculation are not always especially concordant. One of the first things to do in further research would be to compare USEtox and CDV using exactly the same input dataset and also, the necessity to build up a common database to improve the consistency of the impact scores provided by different assessment methods. Otherwise, focusing on the

relevancy of the USEtox method in the context of environmental impact assessment, the case study clearly highlights that this method has drawbacks when compared to CDV: it is more complex and requires also a significant number of entry data. At the same time USEtox is available for evaluation of the entire life cycle, whereas CDV is not. This is not a principal problem with CDV, though, as it could be integrated with LCA databases by the providers of such databases just like USEtox.

5.3 Final thoughts CDV versus USEtox

The results obtained in our case study seem to support the notion that the results obtained with these methods can vary significantly and the methods may thus give a different answer. A more thorough comparison would have to be executed before making any final statements. For example, it should be assessed in how far the results differ if the same data sources (as far as possible) were used in the parametrization. It could be useful in any case to consider using the same robust databases in the future, such as AiiDA. Also, a much larger test set of substances should be used for a comparison.

Since USEtox considers the distribution of a substance in the environment, but CDV does not, it could be relevant to find a solution to add the fate modelling, although CDV follows a conservative approach (100% of the substance flow released in water and bioavailable[3]) that could also (as for ecolabels) be considered acceptable to compare products within the PEF framework. It would be most desirable to perform this fate modelling in a simplified fashion to avoid the subsequent parametrization efforts that are already burden the parametrization of USEtox.

On the other hand, CDV considers the protection of all aquatic species and by the way the trophic food chains, an approach which makes sense from an ecological point of view, but USEtox does not. An evolution of USEtox integrating this approach to derive the aquatic EF appears practicable in a relatively simple manner thanks to the scientific knowledge on ERA.

---

[3] No reduction of the dissolved fraction due to adsorption/desorption to solid particles and dissolved organic carbon or coming from bioaccumulation.

6. CONCLUSIONS AND RECOMMENDATIONS

Assessment of the ecotoxicity of substances is an important part of risk assessment and an integral part of the REACH regulation. In LCA ecotoxicity can also be scored, and it is often among the impact categories that are deemed relevant (based on normalisation) in the PEF pilot studies. The ECETOC taskforce in charge of this report set out to examine the assessment of the impact category of ecotoxicity within LCA, with the perspective of a product assessment instead of a single chemical assessment. The group's composition as a mixed group of ecotoxicologists and LCA practitioners helped shed light on some technical questions as well as foreseeable communication challenges. This chapter summarises the most important findings

Referring to chapter 1 the task force's resources were directed towards the following work items

- Comparison of ecotoxicity assessment in LCA and ecological Risk Assessment
- Comparison and in-depth analysis of tools (USEtox, CDV)
- Influence of LCA best practices on the USEtox ecotoxicity results

The first two bullet points cover mainly technical aspects while the last bullet point has implications on how methods might be used, understood and discussed in the EU context. The discussion in this final chapter intends to cover the technical and contextual aspects.

6.1 Contextual Aspects: Potential Misunderstandings between LCA and RA Experts

LCA is an analytical tool for the (comparative) environmental assessment of products or services and generally covers the entire life cycle, or supply chain, of a product or service. LCA follows the objective to establish the magnitude of environmental impact of a product or service. The tool already established for regulatory purposes is ERA. It evaluates the likelihood of harmful consequences as result of a condition or action on the environment, caused by human activities.

The analysis of freshwater ecotoxicity prescribed for LCA in the context of PEF has significant overlap with the machinery of ERA developed for REACH. Both experts from LCA (PEF) as well as ERA (REACH) will find no difficulty using the USEtox method to generate results. Since they will be interpreted from a different, currently incompatible angle, this is likely to lead to future confusion. The same issue could arise if different regulatory methods have to be applied for the PEF (USEtox) and an Ecolabel (CDV). In the following two paragraphs we address the main communication challenges that arise due to this potential policy overlap.

Both LCA and ERA differ significantly in scope and approach, as described in detail in chapter 2. The key differences that the task force experienced as an example of a mixed group of ERA and LCA experts are the following:

Threshold versus score

ERA is based on the paradigm that there exists a threshold concentration below which there is no effect of a chemical on the environment. Concentrations below the threshold are neglected (i.e. 'safe is safe'). ERA employs a tiered approach in which the information on the threshold concentration (PNEC) and the expected or predicted environmental concentration (PEC) can be refined. As a result, the numeric values of PEC and PNEC represent approximations rather than the 'real' values. In LCA, all emissions, even miniscule, are added in an attempt to calculate the overall 'chemical pressure' on the environment. The result is intended to represent the actual impact on the aquatic environment. In this context 'less is better'. However, these approaches could also be seen as complementary when the objective is to reduce as much as possible an impact beyond the acceptable safety threshold.

Best case approach

In RA, there is an incentive to generate more and higher tier data, through the mechanism of decreasing assessment factors with increasing data richness and by improving the quality of the input data for fate modelling and emission assessment. In LCA, by contrast, absence of data results in a low impact estimate. This is a critical practical shortcoming of LCA that, for the sake of comparability of results, needs to be addressed by agreements on product category rules and minimum data quality requirements.

6.2   Significance of Ecotoxicity Assessment in LCA

In view of its objective (i.e. providing the basis for deciding between two products based on the overall environmental impact) the PEF methodology should be directionally reliable in order to guide consumer decisions and the product development to improvements which optimise the footprint over all relevant impact categories. Questions in this regard are

- When are two product toxicity impacts different from each other?
- How big is the ecotoxicity impact of the product in comparison to the overall ecotoxicity impact?
- How big is the ecotoxicity impact in relation to other impacts?

Question 1 implies that the ecotoxicity impact of individual products can be characterised in such a way that the certainty of the impact estimate is known. Based on this measure of certainty a conclusion can be drawn on whether or not two products are significantly different with regard to their ecotoxicity impact. Answering questions 2 and 3 demands that the global ecotoxicity impact is known. This is true for question 2 in order to find out whether this single product or product category is a significant contributor to the overall ecotoxicity impact. Knowing this global ecotoxicity impact with a sufficient degree of certainty is also a prerequisite to weighting this impact against other impact categories and, finally, to come to proper decisions when it comes to balancing footprint improvements.

All three questions above questions relate to the degree of certainty by which the ecotoxicity impact can be measured or assessed according to the USEtox methodology. In order to improve the understanding of the certainty of the ecotoxicity impact assessment, the ecotoxicity and the greenhouse impact assessments in LCA

are compared to each other step by step. This is to provide an understanding of the degree of certainty of the ecotoxicity assessment in relation to the generally well accepted greenhouse gas impact. Subsequently, the methodology used in USEtox is held against the analysis of the Scientific Committees of the EU commission on existing and newly identified health risks (SCENIHR), on consumer safety (SCCS) and on health and environmental risks (SCHER) (SCENIHR, SCCS, SCHER 2012).

6.2.1   LCA Impact Assessment Comparison: Greenhouse Gas and Aquatic Ecotoxicity

Description

Table 6.1 presents the assessment steps along the impact pathway and lists the key features of each step. Both assessments do not resolve emissions and impact in time or space. In addition, the inventories cover a limited number of emissions. The emissions assessments differ in terms of emission pathways. The greenhouse gases are emitted to the atmosphere only, while the chemical emissions for aquatic ecotoxicity go to water, air and soil. The fate modelling in greenhouse gas assessment assumes homogenous distribution in the atmosphere and takes into account the atmospheric life times of the greenhouse gases (van Loon and Duffy, 2000). As outlined in 2.3, the ecotoxicity assessment applies multimedia fate modelling in order to define the transfer of emissions to atmosphere, water and soil to concentrations in the aquatic compartment. This is achieved by considering advective transport processes and partitioning between the environmental media. In addition, degradation reactions in all compartments are taken into account via half-life times. This requires a whole suite of parameters (see Table 2.2). In addition, the modelling assumes well-mixed homogeneous compartments.

Table 6.1: Comparison of the greenhouse gas and the aquatic ecotoxicity impact assessment as used in LCA

Assessment Step	Greenhouse Gas	Ecotoxicity
Emissions	Ca 140 gases in the inventory Emissions to atmosphere only	Ca 500 substances in the inventory. Emissions to water air and soil. Emissions not spatially / temporally resolved.
Fate modelling	Atmospheric mixing - homogenous distribution in the atmosphere. Degradation of gases in atmosphere.	Multimedia fate modelling – using laboratory data for distribution and environmental reactions. Unit world – not spatially / temporally resolved.
Impact / Midpoint	Sum of radiative forcing of individual emissions. Physical effect.	Sum of incremental extinction of species per substance. Extinction approximated by EC_{50} / PEC. Unit world – not spatially / temporally resolved.

The effect assessment in the greenhouse gas assessment is based on the physical infrared absorbance of the gases and a summation of the radiative forcing of all greenhouse gases. This expresses the heat retained in the atmosphere as a result of the presence of the gases in the atmosphere. Likewise, the effect assessment in ecotoxicity is also based on a summation over all substances. That summation is to approximate aquatic ecosystem damage as a result of the emissions of chemicals.

Evaluation

As outlined above, both greenhouse gas and aquatic ecotoxicity assessment assume that emissions are independent of time and space. In addition, it is assumed in both assessments that the compartments under consideration are well mixed and homogeneous. This assumption appears adequate for greenhouse gas assessment, since atmospheric mixing is rapid (van Loon and Duffy, 2000). It is considered much less adequate for the ecotoxicity assessment taking into account that for instance the emissions of plant protection products are highly seasonal. Similarly, emissions of chemicals which are related to industrial activities or to consumer uses are low in rural areas in comparison with highly industrialised or densely populated areas (Price et al, 2010).

In both greenhouse gas and ecotoxicity impact assessments, additivity of the impact of individual emissions is assumed. This appears adequate for the greenhouse gases, based on the simple physical phenomenon which is modelled (i.e. IR absorbance). The assumption of additivity of ecotoxicological effect for approximating environmental impact is discussed in the ECETOC Technical Report on assessment of the impact of mixtures in the aquatic environment (ECETOC, 2011). This discussion concludes that simple additivity is adequate for lower tier risk assessment, i.e. for assessments which yield a yes/no-answer and which indicate the need for refinement of a risk assessment. However, the examples provided for a more thorough assessment do not rely on predictive modelling but approximate ecological damage at a site-specific level via whole effluent testing or eco-epidemiological investigations on (ECETOC, 2011).

In summary, it can be concluded that both assessments employ a pragmatic simplification. In case of the greenhouse gas impact there appears to be certain degree of matching between the relative simplicity of the modelled system and the modelling applied. In case of the ecotoxicity impact, the high complexity of environmental emission and fate of chemicals and of the relation between chemicals' presence in the environment and ecological damage is addressed with lower tier risk assessment methodology. Hence, the degree of matching of the modelling to the modelled system is lower for ecotoxicity than for the greenhouse gas impact. In consequence, the model results are less certain for ecotoxicity than for greenhouse gases.

Addressing Ecotoxicity Assessment in View of Scientific Committees

Based on the commonalities outlined in 2.7 it is evident that the LCA-aquatic ecotoxicity assessment uses the lower tier risk assessment methodology. This methodology is per se adequate. It is, however, subject to the limitations outlined e.g. by the EU Scientific Committees (EU, 2012). That means the outcome of the calculations underlying the assessments is highly uncertain.

Recently, the scientific advisory committees of the EU commission on Emerging and Newly Identified Health Risks (SCENIHR), on Consumer Safety (SCCS) and on Health and Environmental Risks (SCHER), issued a joint report titled 'Addressing the New Challenges for Risk Assessment' (SCENIHR, SCCS, SCHER, 2012). The report explicitly refers to the 'high uncertainty on the actual consequences of environmental contaminations on the ecosystem structure and functions'. This clearly expresses that the current practice in environmental risk assessment is far from adequately approximating the impact of chemicals on the environment. At the same time, the report concludes that the 'approaches in current use for ecological risk assessment are likely to suffice for regulatory purposes as sufficiently protective for ecosystems.' Hence environmental risk

assessment, through the application of uncertainty/safety/default factors, is effective in screening out low risk cases in order to focus resources on higher risk cases. However, lower tier risk assessment methodology is inapt to yield a realistic representation of the actual impact of chemicals (SCENIHR, SCCS, SCHER, 2012).

The report (2012) also outlines the challenges for improving the risk assessment methodology. The challenges are expressed in view of making risk assessment results more relevant for identifying measures for improvement. This closely relates to Significance Question 2. The respective conclusion is that the 'approaches in current use for ecological risk assessment … lack environmental realism. This entails high uncertainty on the actual consequences of environmental contaminations on the ecosystem structure and functions that has to be addressed by the application of uncertainty/safety/default factors.' The report makes it clear that the major reason for the lack of realism is the overly simplistic approach to assessing ecosystems effects taken in lower tier risk assessments. As outlined above (2.7) the aquatic ecotoxicity assessment in LCA uses the key methodological elements of lower tier ecological risk assessment. Hence, the results of aquatic ecotoxicity assessment in LCA are by analogy highly uncertain.

According to the report (SCENIHR, SCCS, SCHER, 2012) one of the main reasons underlying the uncertainty is the assumption of emissions, environmental transport and degradation being constant. The second major reason lies in the aquatic ecotoxicity assessment in LCA. It is based on an extrapolation from observations on impacts on a few individuals in a few species in the laboratory to express the impact on entire aquatic ecosystems. These two simplistic approximations lead to the uncertainty of the impact assessment. An additional contributor to the uncertainty of the aquatic ecotoxicity assessment is the uncertainty, which is associated with the input data for lower tier risk assessment (see 6.1).

6.2.2   Assessing the Environmental Impact of Mixtures

Overall, the ambition of the aquatic ecotoxicity assessment in LCA in the framework of the PEF-project is to quantify the impact of a chemical mixture on the aquatic ecosystem (see Chapter 2.3). This topic of assessing the impact of a chemical mixture on the aquatic ecosystem has been addressed earlier by ECETOC Report 'Development of Guidance for Assessing the Impact of Mixtures of Chemicals in the Aquatic Environment' (ECETOC, 2011). The major conclusions with regard to prospective assessments are that 'predicting the spatial distribution of chemical exposure in the real-world is difficult and often impossible' and that the principle of concentration addition can be applied in tier 1 prospective assessments of mixture. Given that the USEtox ecotoxicity assessment can be considered a prospective, lower-tier risk assessment of a mixture (or a suite of chemicals), the conclusions of the ECETOC report also hold for USEtox assessments. They imply that the USEtox results rather than expressing actual ecological impact are a relatively gross approximation thereof.

6.2.3   Ecotoxicity Impact Assessment – Database Issues Summary of USEtox Uncertainty Analysis

The EU PEF pilot project uses USEtox to perform aquatic ecotoxicity impact assessment by LCA. As outlined above the results are highly uncertain, primarily due to methodological constraints. Hence, in order to improve the assessment, the sources of uncertainty need to be identified and understood. One source of uncertainty

of the ecotoxicity impact results lies in the principal weakness of the underlying ecological risk assessment methodology.

An additional source of uncertainty of the results of the ecotoxicity impact assessment or the interpretation thereof lies in the LCA database. In order to better understand this uncertainty and to identify improvement options, a deeper look is taken into this database. To that end, the two elements of this data base need to be considered: The life-cycle inventory datasets and the datasets comprising the characterisation factors for the substances.

a) Level of Detail in Life Cycle Inventory datasets

These datasets define the emissions that are related to products and services. Some datasets are very detailed and enumerate a large number of emissions. In general, the level of detail will depend on the scrutiny of the assessor and is not subject to a standardisation. Due to the 'best case' approach that is taken by LCA (refer to chapter 2) this has the consequence that datasets with less details, i.e. a comparatively lower number of material flows (intermediate flows as well as primary emission flows) should have less impact. In RA a lower level of scrutiny would be punished by higher assessment factors, thus giving incentive to add required detail.

b) Missing characterisation factors

As shown in the analysis of the electricity datasets in chapter 5 and as discussed in chapter 2.6, a significant number of substances in the upstream model have no characterisation factors. To make this circumstance visible required significant analysis effort on our side and would normally not be made transparent. The absence of characterisation factors means a contribution of zero to the overall result. It should be worthwhile to establish procedures to make this more transparent and incentivise filling data gaps.

6.3 Conclusion on uncertainty

The above discussion shows that the uncertainty in the ecotoxicity assessment in LCA results from two different factors. One factor is the combination of the deficiencies in the datasets of the life-cycle inventories and the characterisation factors in combination with the fact that these deficiencies typically go unnoticed in LCA practice. As a result, the comparability of two very similar products / services can only be warranted if effort is invested to ensure, that the characterisation factor datasets are complete and of a similar quality and that the life-cycle inventory dataset are complete and with a similar degree of detail.

The second factor is the principal difficulty of assessing ecological impact via the predictive methodology, which is also used in ecological risk assessment. As a result of this, the characterisation factors need to be considered a weak approximation of the actual ecotoxicological impact for each chemical. In addition, the assumed additivity per product / service and over all emissions defined in the LCI datasets are also a gross approximation. For that reason, conclusions on the ecotoxicological impact of a given service / product relative to the entire impact need to be drawn with great caution.

7. WAYS FORWARD

7.1 Reflections on the discussions above

The EU PEF pilot project uses USEtox to perform aquatic ecotoxicity impact by LCA. As outlined above, the results are currently uncertain such that they may not be sufficiently precise for comparing products with each other. Nevertheless, there is a considerable demand for comprehensive evaluations of the environmental impact of products and services. The task force developed options for addressing this need. These are presented in the following.

Hence, in order to improve the assessment, the sources of uncertainty need to be identified and understood. One source of uncertainty of the ecotoxicity impact results lies in the principal weakness of the underlying ecological risk assessment methodology.

An additional source of uncertainty of the results of the ecotoxicity impact assessment or the interpretation thereof lies in the LCA database. In order to better understand this uncertainty and to identify improvement options, a deeper look is taken into this database.

7.1.1 Downstream vs upstream – Need for Including ecotoxicity into LCA

In the down-the-drain product studied in the case study we found upstream contributions to be very minor compared to the downstream counterparts. At the same time, we ask the question of what the upstream contribution would be like if standard emission scenarios such as those defined for ERA (ECHA, 2015) were used. It would be instructive to include these standard scenarios as an option in the datasets covering chemical production in Ecoinvent, to assess whether this has an influence on the relation of the upstream / downstream result.

7.1.2 Freshwater ecotoxicity – Is it relevant for other product categories?

In the case study of a virtual product we assume a quantitative disposal into wastewater, here reasoned to lead to a maximum impact or 'worst-case' scenario. However, the freshwater ecotoxicity assessment using USEtox is not limited to down-the-drain disposal of products but captures the entire life cycle's emissions if needed, by integration with LCA databases. As an example take the production of zinc sulphate, the major freshwater impact of which is generated by upstream during the last production steps by a release of zinc oxide into the atmospheric compartment (fate calculation included in USEtox).

For the worst-case scenario of quantitative disposal into wastewater it should be safe to assume that the downstream part dominates over the upstream creation of materials. In other product categories, however, the impact pattern might be different, even reversed. Considering e.g. water piping (also a PEF pilot!) one could assume that upstream metal production (maybe containing zinc in some applications) and downstream leaching during the use phase (not disposal) might have considerable impacts in the long term. Disposal of slags and other emissions as losses during the recycling of metal products might also play a role.

Even though down-the-drain disposal may be considered to be a worst-case scenario, it is not clear what the proportion of down-the-drain products at the regional scale is compared to all other services and products and which product categories will finally have the highest contribution. A systematic approach for all relevant product categories should be expected to yield further insight into the problem areas and help enhance the estimates in the normalisation projects (Benini et al, 2014; Sala et al, 2014). A catalogue of qualitative descriptors such as available as R.12 (ECHA, 2015) could serve as a guidance to both life cycle assessors and non-experts alike.

7.1.3 Assessing the entire life- cycle – Does it make sense for ecotoxicity?

Ecotoxicity impact as estimated in LCA (through the USEtox methodology) is associated with uncertainty. As outlined in the SCENIHR report (SCENIHR, 2012), significant advancements (both in science and in modelling) are needed in order to reduce the methodological uncertainties in ecotoxicity impact assessment.

The case study results indicate that, in comparison the so-called upstream LC stages, the predominant ecotoxicity impact occurs in the End-of-Life phase. This is the life-cycle stage which is also considered in CDV and in risk assessment. This observation is in agreement with the intuition, because the use of down-the-drain products inadvertently leads to emission of chemicals to water. This study was performed on a virtual product containing seven ingredients chosen for their physico-chemical and ecotoxicological properties. Only two Life cycle stages were compared (Upstream raw material production and End-of-Life). Results suggest that, at least for down-the-drain products, ecotoxicity is mainly driven by End-of-Life stage.

To substantiate this for a broader range of products and services it may be worth the while to compare the ecotoxicity impact of 'down the drain' products with that of other products investigated in the PEF-pilot project in terms of size of impact and the relevant LC-stages. If this is confirmed by looking at other case studies, it may be concluded to go for an approach to address ecotoxicity based on the end-of-life only.

7.2 Ways forward

The EU PEF project is piloting holistic assessments of environmental impacts of products and services. The Task Force presumes that the aquatic ecotoxicity impact assessment is an integral part of these. In view of the discussion above, the Task Force has developed two principal options to assess the aquatic ecotoxicity impact. One is to continue with the PEF approach and to approximate the aquatic ecotoxicity within the LCA framework and thus to address the full life cycle of a product or service. Alternatively, this impact category could be addressed outside of LCA by using approaches that focus on relevant life-cycle stages. The ECETOC Task Force recommends that these options be discussed in a multi-stakeholder workshop involving representatives of JRC as the body initiating the PEF project, representatives of the PEF practitioners, the members of this task force and possibly others. Table 7.1 gives an overview of the options. They will be briefly sketched below in the order of decreasing effort needed for implementing the respective options.

Table 7.1: The two principal options for the way forward with aquatic ecotoxicity impact assessment and their respective sub-options

Principal Option	Address ecotoxicity outside of LCA	Approximate ecotoxicity by LCA
Sub-Option 1	No assessment of Ecotox. in the LCA context: Demonstration of safe use under REACH is sufficient	Business as usual: no changes, just use the current methodology
Sub-Option 2	Use results from Ecolabel ecotoxicity assessment (e.g. CDV) to augment LCA reports	Improve data basis or ecotoxicity assessment (e.g. by use of REACH / HERA data etc.)
Sub-Option 3	-	Improve comparability with ecological risk assessment
Sub-Option 4	-	Improve realism of ecotoxicity assessment – reflect ecology, temporal / spatial variation

7.3 Addressing ecotoxicity by LCA

7.3.1 Improve realism of ecotoxicity assessment

The most advanced options aspire to achieve a degree of realism in ecotoxicity assessment such that the real impact of a product and of all emissions can be estimated to a sufficient degree. To this end, the methodological advancements outlined in the joint report of (SCENIHR 2012) need to be accomplished. In addition, the life-cycle inventories need to be improved as well. The three major suggestions for this are:

- Account for temporal and spatial variability in emissions
- Predicting the extent of concentration changes in time and space
- Improve / replace extrapolation from observations on impacts on a few individuals to consequences for ecosystem structure, processes and services.

7.3.2 Improve data basis – make life-cycle based ecotoxicity assessments comparable among each other

Since the above option involves a significant research effort, it is not likely to be implemented soon, i.e. within the next decade. For that reason, a first step to improve the current methodology is to improve the database used in the make life-cycle based ecotoxicity assessments and to improve the homogeneity of data quality. Investing effort into this will make the assessment results comparable to each other such that ecotoxicity comparisons of products / services along the entire life-cycle become more meaningful. In that regard it needs to be noted, that a wealth of data has become and continues to become available through EU chemicals legislation.

Use of data collected for REACH

Since the enforcement of REACH in 2006, a huge amount of new experimental toxicity data was generated for the ongoing REACH registrations. Furthermore, the already available data was re-evaluated according to current scientific knowledge and following official guidelines for quality requirements. Consequently, data

generated in the scope of REACH should thus be useful in filling in data gaps that exist in USEtox nowadays. A large body of physical-chemical and degradation data have become available through the REACH registrations. These are available for improving the quality of the characterisation factors and in expanding the number of datasets.

In order to capitalise on the REACH data for LCA, the following needs to be considered in the discussion of this option. With the chronic EC_{50} being the reference point for USEtox this necessitates a reinterpretation of raw data, which is a very laborious and time consuming endeavour.

Data availability. USEtox uses an effect-based indicator based on the use of chronic EC_{50}1 values to derive the ecotoxicological effect factor for the respective substance (Huijbregts et al, 2010). The choice of chronic values seems logical as LCA typically deals with marginal concentration increases in the 'model' environment. Therefore, emissions will mostly give rise to potentially chronic effects that are hardly covered in acute toxicity studies that usually deal with mortality as endpoint (Larsen and Hauschild, 2007). The decision to use the (chronic) EC_{50} value was based on the robustness of the EC_{50} because in general this value has the smallest confidence interval compared to much lower ECx1 values (e.g. the EC_{10} value; Payet, 2004; Forbes and Forbes, 1993; Rivière, 1998). NOEC values are completely disregarded due to the fact that a NOEC2 value is dependent on the choice of the test concentration and no confidence intervals can be calculated. From a statistical point of view this strategy seems to be reasonable, however, from an applied practitioner perspective it seems hard to understand why chronic EC_{50} values are the values of choice.

Acute to Chronic Extrapolation. The most important aspect is that chronic EC_{50} are hardly reported in experimental toxicity studies. Therefore, the user of USEtox has only the choice to derive the chronic EC_{50} value by applying an acute-to-chronic extrapolation from the acute EC_{50} value which is regularly derived in aquatic toxicity studies. By default, an assessment factor of 2 (10 for metals) is suggested to be applied on the acute species EC_{50} to derive the chronic species EC_{50}. NOEC values or EC_{10} values from reliable chronic toxicity studies are not taken into account. However, the choice of an acute-to-chronic extrapolation factor of 2 seems rather arbitrary as the extrapolation is highly dependent on the mode of action of the specific compound. The ECETOC TR No. 91 lists several acute to chronic ratios based on different modes of action (narcotic, inorganic, polar narcotic, reactive, and specific acting). Although this work concentrated on deriving a chronic NOEC value (not a chronic EC_{50} value as used in USEtox) from an acute EC_{50} value, it could be clearly shown that the acute to chronic ratios are highly dependent on the mode of action. Therefore, a default factor of 2 (10 for metals) as used in USEtox does not seem to be the best choice. Further research is needed to address this issue and it would be desirable to at least take the mode of action of the compound into account if an acute to chronic extrapolation is really needed.

Use of Existing Dose-Response Information. Another topic that needs further attention is the non-use of NOEC and/or EC_x (e.g. EC_{10}) values from reliable chronic toxicity studies. As mentioned before these values are usually derived in aquatic chronic toxicity studies and it would make sense to include these values in the derivation of the effect factor in USEtox without further extrapolation. The choice of the chronic EC_{50} value was based on the robustness of the EC_{50} and the lower confidence interval compared to EC_x (e.g. EC_{10}) values. However, although the confidence interval of EC_x values is usually higher compared to EC_{50} values it is highly dependent on the individual test substance and the experimental design. Furthermore, NOEC values derived from reliable experimental studies deliver valuable information and are definitely to be preferred over

extrapolated data from acute studies. Another possibility to derive chronic EC_{50} values is a complete re-evaluation of the raw data of the experimental study itself. If the raw data is available and the study design allows the derivation of a chronic EC_{50} value this would be an option to derive a scientifically sound value without the need to extrapolate from acute data. However, for practical reasons this option is not favoured as it would mean an additional workload that could be avoided if other options, i.e. NOECs, EC_{10}, were possible.

Still, a successful current use case exists for the reinterpretation of the raw data (dose-response curves) such as practised currently in the update of the characterisation factors for the metals zinc, copper, cadmium, nickel, cobalt, aluminium, antimony, lead, iron and molybdenum in USEtox by the metals associations.

7.3.3   Increasing comparability with ecological risk assessment

Increasing the comparability of the ecotoxicity assessment with ecological risk assessment is another option. It can be implemented by changing the ecotoxicity reference from the geometric mean-based effect assessment with the use of the data for the most sensitive species (or trophic level). This ecotoxicity reference is used in ecological risk assessment and e.g. in the CDV-method. The use of this reference would thus bring methodological harmonisation. It can be achieved by replacing chronic EC_{50} values to with other – more practical, real-life – options (e.g. NOEC/EC_{10} that are actually derived in aquatic experimental studies) for the derivation of the effect factor. These data have become available through REACH. The authors recognise the attempt to use the most robust value for modelling purposes. However, the uncertainty that is introduced by extrapolation from acute EC_{50} values without further taking into account the mode of action of the compound does not seem the best choice. Although this task force was not able to further address these issues it would be desirable to evaluate it in further works as this is a critical aspect not only for the outcome of the modelling approach with USEtox but also the general use of data that was prepared for current regulatory works.

7.3.4   Continue with current approach and understand degree of uncertainty

As outlined in 6.2.4, the data in the life-cycle inventory may be of quite different quality. In addition, the database for the characterisation factors, even though it has grown significantly over recent years still has gaps. These gaps and quality differences are likely to go undetected in a typical LCA which uses the data as they are available in the LCA databases. Hence, in order to continue the typical current practice of LCA of using the datasets from the currently available databases a quantitative understanding needs to be developed of the degree of uncertainty of the entire method. Based on this significance, criteria may be derived for judging if two products based on their impact scores are actually different from each other with regard to ecotoxicity.

7.4   Address Ecotoxicity outside of LCA

7.4.1   Accept Safe Use as Negligible Impact

Although this may seem like a provocative suggestion, it should be considered a serious option. The REACH regulation with its process regulates the use of chemicals to a level where the risk for the environment is

considered acceptable and there is minimal environmental impact as supported by scientific methods. Beyond this goal, the benefit that LCA could add here is the 'less is better' paradigm. In the absence of external references this can lead to the point that effort is invested in optimising systems that do not require further optimisation.

7.4.2   CDV: Establish ecotoxicity impact outside LCA

CDV is the method currently employed in the EU ecolabel to detergent and cosmetic products (EC, 2014a; Nordic Ecolabelling, 2010). CDV is simple to apply for comparison of down-the drain consumer products in the range of cosmetics and laundry detergents based on the two key environmental parameters (biodegradation and aquatic ecotoxicity) required and the fact that for many ingredients the parameters are already tabulated. As shown in the cases study where the down-the-drain stage of the life cycle is the by far biggest contributor to the impact, it may be worthwhile discussing, for certain products, whether a CDV assessment may be useful as ecotoxicity complement to an LCA, which does not include this impact category.

7.5   Next Steps

This report provides a scientific evaluation of the USEtox method, currently the leading method for calculating toxicity impacts in LCA. In addition, it has investigated how USEtox relates to chemical risk assessment methodology and to the critical dilution volume as additional environmental evaluation schemes for chemicals or chemical products.

The third remit of the task force was to provide guidance on the scientific relevance and interpretation of USEtox results in the context of chemical impact assessment and selection of chemical-based (manufactured) products. In this regard, the present report has deepened the understanding of the uncertainty of aquatic ecotoxicity impact. While the extent of uncertainty cannot be quantified at present, it is clear for the task force that a discussion is needed on how to go forward with the aquatic ecotoxicity impact. Since this is not a scientific question, it is beyond the task force remit to provide an answer. Instead, the task force recommends a multi-stakeholder discussion of this issue and proposes to have a workshop in this issue. Ideally, the workshop attendants should include representatives of JRC as the body initiating the PEF project, representatives of the PEF practitioners, the members of this task force and possibly others.

ABBREVIATIONS

AIIDA	Aquatic Impact Indicators Database
AISE	International Association for Soaps, Detergents and Maintenance Products
B2B	Business-to-business
B2C	Business-to-consumer
BIT	Benzisothiazolinone
CDV	Critical dilution volume
CF	Characterisation factor
CTU	Comparative toxic unit
DALY	Disability adjusted life year
DF	Degradation factor
DID	Detergent ingredient database
EC_{10}; EC_{50}	Effective Concentration, 10%; 50%
EF	Effect factor
E-LCA	Environmental LCA
E(L)Cx	x% Effect (Lethal) Concentration
ECA	Ecotoxicological classification factor
ELCD	European Reference Life Cycle Database
EPD	Environmental product declaration
ERA	Environmental risk assessment
ESC	Environmental safety check
EU	European Union
EUSES	The European Union System for the Evaluation of Substances
FF	Fate factor

FU	Functional unit
GHS	Global harmonised system
HC_{50}	
ILCD	International reference life cycle data system
IS	Impact score
JRC	Joint Research Centre
LAS	Linear alkylbenzene sulphonate
LCA	Life cycle assessment
LCC	Life cycle costing
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LF	Loading factor
NOEC	No observed effect concentration
OEF	Organisation environmental footprint
PAF	Potentially affected fraction of species
$PDF.m^2.y$	Potentially disappeared fraction of species on 1 m^2 during one year because of pressure induced on the considered ecosystem
PEC	Predicted environmental concentration
PEF	Product environmental footprint
PEFCR	Product environmental footprint category rules
PNEC	Predicted no effect concentration
QMRA	Quantitative microbial risk assessment
QSAR	Quantitative structure-activity relationship
RA	Risk assessment
RCR	Risk characterisation ratio

REACH	Registration, evaluation, authorisation and restriction of chemicals
RMM	Risk management measure
S-LCA	Social LCA
SCCP	(EU) Scientific Committee on Consumer Products
SCCS	(EU) Scientific Committee on Consumer Safety
SCENIHR	(EU) Scientific Committee on Emerging and Newly Identified Health Risks
SCHER	(EU) Scientific Committee on Health and Environmental Risks
SCP/SIP	(EC) Sustainable Consumption and Production and Sustainable Industrial Policy
SETAC	Society of Environmental Toxicology and Chemistry
SF	Safety factor
SMGP	Single Market for Green Products
SSD	Species sensitivity distribution
TF	Toxicity factor
TRA	Targeted risk assessment
TSC	The Sustainability Consortium
UNEP	United Nations Environment Programme
UPR	Unit process raw
XF	Exposure factor

BIBLIOGRAPHY

AFNOR Certification. 2011. Référentiel de certification de la marque NF Environnement « Produits de Nettoyage ». NF438. 2009, updated in 2011. http://cdn.afnor.org/download/reglements/FR/REGNF438.pdf

AiiDA. 2014. An intuitive Ecotoxicity Database for Risk Management and LCA. Last updated: 10-Jun-2014. Consulted in February 2016. http://aiida.tools4env.com/

AISE. 2015. Unpublished PEF screening report in the context of the EU Product Environmental Footprint Category Rules (PEFCR) Pilots: Household Heavy Duty Liquid Laundry Detergents (HDLLD) for machine wash. International Association for Soaps, Detergents and Maintenance Products (AISE), Brussels, Belgium.

Askham C. 2012. REACH and LCA-methodological approaches and challenges. Int J LCA 17(1):43–57.

Bare JC, Norris GA, Pennington DW, McKone TE. 2003. TRACI, The Tool for the Reduction and Assessment of Chemical and other environmental Impacts. J Ind Ecol 6(3-4): 49-78.

Benini L, Mancini L, Sala S, Manfredi S, Schau EM, Pant R. 2014. Normalisation method and data for Environmental Footprints. Report EUR 26842 EN. European Commission, Joint Research Centre, Institute for Environment and Sustainability, Publications Office of the European Union, Luxemburg. http://ec.europa.eu/environment/eussd/smgp/pdf/JRC_Normalisation_method_and_data_EF_web.pdf

Berna JL, Cavalli L, Renta C. 1995. A Life-cycle inventory for the Production of Linear Alkylbenzene Sulphonates in Europe. Tenside Surf Det 32(2):122-127.

Brandes LJ, den Hollander H, van de Meent D. 1996. SimpleBox 2.0: a nested multimedia fate model for evaluating the environmental fate of chemicals. RIVM report 719101029. RIVM, National Institute of Public Health and the Environment, Bilthoven, The Netherlands. http://www.rivm.nl/bibliotheek/rapporten/719101029.pdf

EC. 2001a. European Commission Directive 2001/82/EC of the European Parliament and of the Council of 6 November 2001 on the Community code relating to veterinary medicinal products (OJ L 311, 28/11/2001, pp 1-66). (Consolidated version: 18/7/2009). http://ec.europa.eu/health/files/eudralex/vol-5/dir_2001_82/dir_2001_82_en.pdf

EC. 2001b. European Commission Directive 2001/83/EC of the European Parliament and of the Council of 6 November 2001 on the Community code relating to medicinal products for human use (OJ L 311, 28.11.2001, pp 67).

EC. 2007. Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18th December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC. OJ L 136 of 29.5.2007, Luxemburg.

EC. 2008. European Commission Directive 91/414/EEC – evaluation, authorisation, approval of active substances at EU-level and national authorisations of PPPs, Brussels Belgium. The placing of plant protection products on the market (until June 2011)

EC. 2010. ILCD handbook (International Reference Life Cycle Data System) —General guide for Life Cycle Assessment—Detailed guidance. EUR 24708 EN. European Commission, Joint Research Centre, Institute for Environment and Sustainability, 1st ed. Publications Office of the European Union, Luxemburg, 398 pp.

EC. 2013a. 2013/179/EU: Commission Recommendation of 9 April 2013 on the use of common methods to measure and communicate the life cycle environmental performance of products and organisations. Annex II: Product Environmental Footprint (PEF) Guide. OJ L 124, Volume 56, 4 May 2013. http://eur-lex.europa.eu/JOHtml.do?uri=OJ:L:2013:124:SOM:EN:HTML

EC. 2013b. Application pack for the Ecolabel. Application form and guidance document for laundry detergents. Commission Decision of 28 April 2011 on establishing the ecological criteria for the award of the EU Ecolabel for laundry detergents. 29 pp. http://ec.europa.eu/environment/ecolabel/documents/User_manual_laundry.pdf

EC. 2014a. EU Ecolabel rinse-off cosmetics user manual. Commission Decision for the award of the EU Ecolabel for rinse-off cosmetics (2014/893/EU), 77 p. http://ec.europa.eu/environment/ecolabel/documents/User_manual_cosmetics.pdf

EC. 2014b. Detergents Ingredients Database (DID-list) Part A. List of ingredients version 2014.1. http://ec.europa.eu/environment/ecolabel/documents/did_list/didlist_part_a_en.pdf

EC. 2014c. Detergents Ingredients Database. Version 2014.1. DID-list Part B. http://ec.europa.eu/environment/ecolabel/documents/did_list/didlist_part_b_en.pdf

ECETOC. 2003. Aquatic Hazard Assessment II. Database. Technical Report No. 91. European Centre for Ecotoxicology and Toxicology of Chemicals, Brussels, Belgium.

ECETOC. 2011. Development of guidance for assessing the impact of mixtures of chemicals in the aquatic environment. Technical Report No. 111. European Centre for Ecotoxicology and Toxicology of Chemicals, Brussels, Belgium.

ECHA. 2008. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.10: Characterisation of dose [concentration]-response for environment. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/documents/10162/13632/information_requirements_r10_en.pdf

ECHA. 2011, 2016. Disseminated REACH registration dossier of acrylic acid (EC 201-177-9, CAS 79-10-7). Full registration type, 1,000,000-10,000,000 tonnes per annum, first published: 04-Mar-2011, last updated: 14-Oct-2016. Consulted in October 2016. http://www.echa.europa.eu/fr/web/guest/registration-dossier/-/registered-dossier/15803

ECHA. 2015. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.12: Use description, v3.0. European Chemicals Agency, Helsinki, Finland. http://echa.europa.eu/documents/10162/13632/information_requirements_r12_en.pdf

ECHA. 2016. Guidance on Information Requirements and Chemical Safety Assessment. Chapter R.16: Environmental exposure assessment, v3.0. European Chemicals Agency, Helsinki, Finland. https://echa.europa.eu/documents/10162/13632/information_requirements_r16_en.pdf

Eskeland MB, Svanes E. 2004. The harmonised Detergent Ingredient Database ("DID-list") for eco-labelling. Ecolabelling Norway. http://www.svanemerket.no/Documents/Kriterier%20mm/DID_Final_report_504_Engelsk.pdf

EU. 2012. Regulation (EU) No 528/2012 of the European Parliament and of the Council of 22 May 2012 concerning the making available on the market and use of biocidal products. OJ L 167 of 27.6.2012, Luxemburg. The EU Biocides Regulation 528/2012 (EU BPR) was consulted at http://www.hse.gov.uk/biocides/eu-bpr/index.htm

EU. 2014. Commission Decision 2014/893/EU of 9 December 2014 establishing the ecological criteria for the award of the EU Ecolabel for rinse-off cosmetic products. OJ L 354 of 11.12.2014, Luxemburg, pp 47-61. http://data.europa.eu/eli/dec/2014/893/oj

EU TGD Part II. 2003. Technical Guidance Document on Risk Assessment Part II. European Chemicals Bureau, Institute for Health and Consumer Protection Ispra, Italy.

European Ecolabel. 2011. Revision of Ecolabel Criteria for Laundry Detergents 2008-2010. Background report. Prepared by Ecolabelling Denmark. http://ec.europa.eu/environment/ecolabel/documents/Laundry%20Detergents%20technical%20report.pdf

Forbes TL, Forbes VE. 1993. A critique of the use of distribution-based extrapolation models in ecotoxicology. Funct Ecol 7:249-254.

Frischknecht R, Jungbluth N, Althaus HJ, Doka G, Dones R, Heck T, Hellweg S, Hischier R, Nemecek T, Rebitzer G, Spielmann M. 2005. The ecoinvent database: Overview and methodological framework. Int J LCA 10(1):3-9.

Frischknecht R, Steiner R, Jungbluth N. 2008. Methode der ökologischen Knappheit – Ökofaktoren 2006, Öbu und Bundesamt für Umwelt, Bern, Switzerland.

Gleerup Ovesen R, Eskeland MB, Axelsson L. 2013, adjusted in 2014. Revision of the harmonised Detergent Ingredient Database. Final report. pp 52.

Harder R, Holmquist H, Molander S, Svanström M, Peters GM. 2015. Review of environmental assessment case studies blending elements of risk assessment and life cycle assessment. Environ Sci Technol 49(22):13083–13093.

Hauschild MZ, Huijbregts MAJ. 2015. Life Cycle Impact Assessment. Springer, Netherlands, pp 345.

Heijungs R, Suh S. 2002. The Computational Structure of Life Cycle Assessment. Springer, Netherlands, pp 243.

Heijungs R, Guinée JB, Huppes G, Lankreijer RM, Udo de Haes HA, Wegener Sleeswijk A. 1992. Environmental Life Cycle Assessment of Products. Guide. Leiden, Centre of Environmental Science, 96 pp.

Hischier R, Classen M, Lehmann M, Scharnhorst W, eds. 2007. Life cycle inventories of Electric and Electronic Equipment: Production, Use and Disposal. Ecoinvent report No. 18. Swiss Centre for Life Cycle Inventories, Dübendorf, Switzerland.

Huijbregts MAJ, van Zelm R, Rombouts L, Ragas A, Struijs J, Goedkoop M, Heijungs R, Harbers J, Wintersen A, Posthuma L, Hendriks J, van de Meent D. 2009. Chapter 7 - Toxicity. In: Goedkoop M, Heijungs R, Huijbregts MAJ, Struijs, J, De Schryver A, van Zelm R. ReCiPe 2008, A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level. First edition. Report I: Characterisation.

Huijbregts M, Hauschild M, Jolliet O, Margni M, McKone T, Rosenbaum RK, van de Meent D. 2010. USEtoxTM User manual. USEtoxTM User manual. http://www.USEtox.org/support/tutorials-manuals

Huijbregts M, Hauschild M, Margni M, Jolliet O, McKone T, van de Meent D, Rosenbaum R. 2015a. USEtox® 2.0 Manual: Inorganic Substances (Version 2). USEtox® Manual: Inorganic Substances. http://www.USEtox.org/model/download/USEtox2.0

Huijbregts M, Margni M, Hauschild M, Jolliet O, McKone T, Rosenbaum RK, van de Meent D. 2015b. USEtox® User manual (Version 2). USEtox® User manual. http://www.USEtox.org/support/tutorials-manuals

Huijbregts M, van de Meent D, Margni M, Jolliet O, Rosenbaum R, McKone T, Hauschild M. 2015c USEtox® 2.0 MANUAL: ORGANIC SUBSTANCES (Version 2). USEtox® Manual: Organic Substances. http://www.USEtox.org/model/download/USEtox2.0

ISO 14040. 1997, revised in 2006. Environmental management – Life cycle assessment – Principles and framework. International Organization for Standardization, Geneva, Switzerland.

ISO 14044. 2006, revised in 2016. Environmental management – Life cycle assessment – Requirements and guidelines. International Organization for Standardization, Geneva, Switzerland.

Jolliet O, Margni M, Charles R, Humbert S, Payet J, Rebitzer G, Rosenbaum R. 2003. IMPACT 2002+: A New Life Cycle Impact Assessment Methodology. Int J LCA 8(6):324-330.

JRC-IES. 2011. European Commission-Joint Research Centre — Institute for Environment and Sustainability: International Reference Life Cycle Data System (ILCD) Handbook — Recommendations for Life Cycle Impact Assessment in the European context. First edition November 2011. EUR 24571 EN. Publications Office of the European Union, Luxemburg. http://eplca.jrc.ec.europa.eu/uploads/ILCD-Recommendation-of-methods-for-LCIA-def.pdf

JRC-IHCP. 2010.European Union Risk Assessment Report – Zinc Metal (EUR 24587). Munn S, Aschberger K, Olsson H, Pakalin S, Pellegrini G, Vegro S, Paya Perez AB, eds. European Commission – Joint Research Centre – Institute for Health and Consumer Protection. Publications Office of the European Union, 695 pp. http://publications.jrc.ec.europa.eu/repository/handle/JRC61245

Kemna R, van Elburg M, Li W, van Holsteijn R. 2005. MEEUP (Methodology Study Eco-design of Energy-using Products) – Methodology Report. Final version 28-11-2015. European Commission, Brussels, Belgium.

Klimisch HJ, Andreae M, Tillmann U. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. Regul Toxicol Pharmacol 25(1):1-5.

Larsen HF, Hauschild MZ. 2007. GM-troph: a low data demand ecotoxicity effect indicator for use in LCIA. Int J LCA 12(2):79–91.

Martz P, L'Haridon J, Chenèble JC, Campion JF, Cuenot L. 2015. Environmental labelling of rinse-off cosmetic products: comparing CDV and USEtox using the same ecotoxicity factor. Poster presented at 25th SETAC (Society of Environmental Toxicology and Chemistry) Europe Congress, Barcelona, Spain.

Medyna G, Boyano A. 2014. Toxicity to aquatic organisms in the EU Ecolabel criteria for detergents and rinse-off cosmetic products. Document drafted to support EUEB meeting of June 2014, Sevilla, Spain.

Nitschke L, Malcomber I, Tibazarwa C, Steber J. 2007. Is the EU Ecolabel DID list a useful environmental evaluation tool for detergent-like consumer products? Tenside Surf Det 44(3):155-15.

Nordic Ecolabelling. 2010. Nordic Ecolabelling of Cosmetic products. Version 2.11 • 12 October 2010 – 30 June 2017. http://www.nordic-ecolabel.org/criteria/product-groups/

Nordic Ecolabelling. 2013. Nordic Ecolabelling of Cleaning products. Version 5.2 • 13 March 2013 – 31 March 2017. http://www.nordic-ecolabel.org/criteria/product-groups/?p=2

Nordic Ecolabelling. 2015. Criteria document for Nordic Ecolabelling of Cosmetic products. 090 Cosmetic products, version 2.10, 4 June 2015, 25 pp.

OECD. 1992. Guidelines for the Testing of Chemicals. Ready Biodegradability. Test No. 301. OECD Publishing. Organisation for Economic Co-operation and Development, Paris, France.

OECD. 2004. OECD Series on Testing and Assessment No. 45: Guidance document on the use of multimedia models for estimating overall environmental persistence and long-range transport. ENV/JM/MONO(2004)5. Organisation for Economic Co-operation and Development, Paris, France.

OECD. 2014. Guidelines for the Testing of Chemicals. Degradation and Accumulation. Test No. 310: Ready Biodegradability - CO2 in sealed vessels (Headspace Test). OECD Publishing. Organisation for Economic Co-operation and Development, Paris, France.

Olsen SI, Christensen FM, Hauschild M, Pedersen F, Larsen HF, Tørsløv J. 2001. Life cycle impact assessment and risk assessment of chemicals — a methodological comparison. Environ Impact Assess Rev 21(4):385-404.

Payet J. 2004. Assessing Toxic Impacts on Aquatic Ecosystems in Life Cycle Assessment (LCA). PhD thesis No. 3112 (2004). EPFL, Lausanne, Switzerland.

Pickup JA, Dewaele J, Furmanski NL, Kowalczyk A, Luijkx GCA, Mathieu S, Stelter N. 2016. A risk-based, product-level approach for assuring aquatic environmental safety of cleaning products in the context of sustainability: the Environmental Safety Check (ESC) scheme of the A.I.S.E. Charter for Sustainable Cleaning, Integr Environ Assess Manag, DOI 10.1002/ieam.1764.

Price OR, Hughes GO, Roche NL, Mason PJ. 2010. Improving emission estimates of home and personal care products ingredients for use in EU risk assessments. Integr Environ Assess Manag 4:674-681.

Reihlen A, Bahr T, Boegi C, Dobe C, May T, Verdonck F, Wind T, Zullo L, Tolls J. 2016. SPERCS—A Tool for environmental emission estimation. Integr Environ Assess Manag 12(4):772-781.

Rivière JL. 1998. Evaluation du risque écologique des sols pollués. Lavoisier, Paris, France, 228 pp.

Rohe DMM, Wolf HU. 2007. Zinc Compounds. Ullmann's Encyclopedia of Industrial Chemistry, 7th ed. Wiley-VCH Verlag, Germany.

Rosenbaum RK, Bachmann TM, Swirsky Gold L, Huijbregts MAJ, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni M, McKone TE, Payet J, Schuhmacher M, van de Meent D, Hauschild MZ. 2008. USEtox— the UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in life cycle impact assessment. Int J LCA 13(7):532-546.

Sala S, Benini L, Mancini L, Ponsioen T, Laurent A, van Zelm R, Stam G, Goralczyk M, Pant R. 2014. Methodology for building LCA-compliant national inventories of emissions and resource extraction. European Commission, Joint Research Centre, Institute for Environment and Sustainability, Publications Office of the European Union, Luxemburg. http://bookshop.europa.eu/en/methodology-for-building-lca-compliant-national-inventories-of-emissions-and-resource-extraction-pbLBNA26871/

SCENIHR, SCCS, SCHER. 2012. Preliminary report on Addressing the New Challenges for Risk Assessment, 8 October 2012. European Commission, Scientific Committee on Emerging and Newly Identified Health Risks, Scientific Committee on Consumer Safety, Scientific Committee on Health and Environmental Risks. http://ec.europa.eu/health/scientific_committees/emerging/docs/scenihr_o_037.pdf

Steen B. 1999a. A Systematic approach to environmental priority strategies in product development (EPS). Version 2000 – General system characteristics. CPM report 1999:4. Chalmers University of Technology, Gothenburg, Sweden.

Steen B. 1999b. A Systematic approach to environmental priority strategies in product development (EPS). Version 2000 – Models and data of the default method. CPM report 1999:5. Chalmers University of Technology, Gothenburg, Sweden.

Tørsløv J, Hauschild MZ, Rasmussen D. 2005. Ecotoxicity. In Potting J, Hauschild MZ, eds, Spatial differentiation in Life Cycle impact assessment – The EDIP2003 Methodology. Environmental News no. 80. Danish Ministry of the Environment, Environmental Protection Agency, Copenhagen, Denmark.

UNEP. 1999. Technical Workbook on Environmental Management Tools for Decision Analysis: Technical Papers and Workbook. United Nations Environment Programme, Geneva, Switzerland.

van Leeuwen CJ, Vermeire TG, eds. 2007. Risk assessment of chemicals: an introduction. Springer, The Netherlands, pp 511–551.

van Loon GW, Duffy SJ. 2000. Environmental chemistry. A global perspective. Oxford University Press, New York, USA, pp 23-28.

van Zelm R, Huijbregts MAJ, Harbers JV, Wintersen A, Struijs J, Posthuma L, van de Meent D. 2007. Uncertainty in msPAF-based ecotoxicological effect factors for freshwater ecosystems in Life Cycle Impact Assessment. Integr Environ Assess Manag 3(2):203-210.

WHO. 1996. Linear alkylbenzene sulfonates (LAS) and related compounds. IPCS – Environmental Health Criteria 169, World Health Organization, Geneva, Switzerland.
http://www.inchem.org/documents/ehc/ehc/ehc169.htm

Zah R, Hischier R. 2007. Life Cycle Inventories of Detergents. Final report Ecoinvent data v2.0, No. 12. Swiss Centre for Life Cycle Inventories, Dübendorf, Switzerland.

MEMBERS OF THE TASK FORCE

Nikolaj Otte (Chair)   Henkel
Manager Life Cycle Assessment and Sustainability   D - Düsseldorf

Michiel Claessens *   Chemours
Regulatory Ecotoxicologist   B - Kallo

Chris Cooper   International Zinc Association
Assistant Manager, Environmental Affairs   B - Brussels

Robert Hoke   DuPont
Principal Environmental Toxicologist   USA - Newark, DE

Henry King   Unilever
Science & Technology Leader - Sustainability   UK - Bedford

Jacques L'Haridon   L'Oréal Research & Innovation
Head of Predictive Environmental Methods and Evaluations   F - Aulnay-sous-Bois

Frederic Palais   Solvay
Regulatory Ecotoxicologist   F - Saint Fons

Florian Schmidt   BASF
Regulatory Ecotoxicologist   CH - Langnau am Albis

Diederik Schowanek   P&G, Belgium
Principal Environmental Scientist   B - Strombeek-Bever

Thomas Wolf **   L'Oréal Research & Innovation
Associate Director - Head of Environmental Safety   F - Asnières-sur-Seine Cedex

Malyka Galay Burgos (Scientific Secretary) ***   ECETOC
Environmental Sciences Manager   B - Brussels

* Resigned on August 29, 2016
** Left L'Oréal end of September 2016
*** Left ECETOC July 2016

MEMBERS OF THE SCIENTIFIC COMMITTEE

(Peer Review Committee)

MEMBERS OF THE SCIENTIFIC COMMITTEE (cont'd)

ECETOC published Reports

The full catalogue of ECETOC publications can be found on the ECETOC website:
http://www.ecetoc.org/publications

ECETOC published Reports