National Institute for Public Health
and the Environment
Ministry of Health, Welfare and Sport

From risk assessment to environmental impact assessment of chemical substances

Methodology development to be used in socio-economic analysis for REACH

RIVM report 601353002/2012

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Colophon

J.K. Verhoeven
J. Bakker
Y. Bruinen de Bruin
E.A. Hogendoorn
J.A. de Knecht
W.J.G.M. Peijnenburg
L. Posthuma
J. Struijs
T.G. Vermeire
H.J. van Wijnen
D. de Zwart

Contact:
Julia Verhoeven
Expertise Centre for Substances
julia.verhoeven@rivm.nl

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Abstract

Methodology for the determination of environmental impacts of chemicals

A methodology is proposed to determine and compare expected environmental effects of chemical compounds. This provides information on the relative environmental benefits when a hazardous substance would be replaced by a less harmful alternative. The study focuses on the environmental damage of both the hazardous compound and its alternative(s). In comparison to previous studies, the proposed methodology makes it relatively simple to determine and compare environmental impacts.

The EU legislation REACH (Registration, Evaluation Authorisation and restriction of Chemicals) came into force in 2007. Authorisation and Restriction are two tools that REACH provides to ban or replace a substance that is regarded as dangerous to humans and / or the environment. In case of a ban or use limitation of a chemical, REACH proposes to estimate broader impacts of the ban by means of a so-called socio-economic analysis (SEA). In an SEA, for example, the reduced damage to humans and the environment of switching to an alternative can be weighed against the socio-economic costs of the switch. This project focuses on a methodology comparing environmental effects (environmental damage) which provides the required input for part of the socio-economic analysis.

The methodology consists of a tiered approach to account for gross and refined problem definitions as well as data limitations. Approaches used are based on the type of compound(s), data availability and the ultimate goal of the analysis. The methodology also provides a framework on dealing with uncertainties.

The usefulness of the developed methodology is tested on the basis of three case studies of very different substances: (1) the historic replacement of nonylphenol (surfactant) in detergents by alcohol ethoxylates, (2) the replacement of zinc gutters by PVC gutters, and (3) the replacement of the fire retardant HBCDD in insulating building material by two alternative flame retardants.

Keywords:
Environmental impact assessment, chemical substances, socio-economic analysis, restriction, authorisation, REACH

Rapport in het kort

Methodologie voor bepalen van de milieu-impacts van chemische stoffen

Dit rapport stelt een methodologie voor waarmee verwachte milieu-effecten van chemische stoffen onderling kunnen worden vergeleken. Dit levert inzicht op in de relatieve milieuwinst die kan worden behaald als schadelijke stoffen worden vervangen door minder schadelijke alternatieven. Centraal staat de milieuschade van zowel de bestaande stof als het alternatief. Ten opzichte van eerdere verkenningen geeft deze studie een methodologie waarmee milieuschade relatief eenvoudig kan worden bepaald en vergeleken.

In 2007 is de Europese wetgeving REACH (Registration, Evaluation Authorisation and restriction of CHemicals) ingevoerd. Restrictie en Autorisatie zijn de twee instrumenten van REACH om een stof die op grond van de huidige kennis als gevaarlijk voor mens en/of milieu wordt beschouwd, uit te faseren en te vervangen door een alternatief. REACH schrijft voor dat de gevolgen van een verbod in bredere zin dan alleen een risicoanalyse, worden weergegeven, namelijk via een zogenoemde socio-economische analyse. Hierin kan de verminderde schade aan mens en milieu bijvoorbeeld worden afgewogen tegen de kosten die een overschakeling op een alternatief met zich meebrengt. De ontwikkelde methodologie richt zich alleen op milieu-effecten als onderdeel van een socio-economische analyse.

De methodologie bestaat uit een getrapte analyse, waarmee kan worden gekozen voor de manier en het detailniveau waarop de methodologie wordt uitgevoerd. Dit gebeurt op basis van het type stof, de databeschikbaarheid en het uiteindelijke doel van de analyse. Tevens geeft de methodologie een raamwerk hoe bij dergelijke analyses om te gaan met onzekerheden.

De bruikbaarheid van de ontwikkelde methodologie is getest met behulp van drie voorbeeldstudies van zeer verschillende stoffen. Het betreft (1) de vervanging van nonylfenolen (surfactanten) in wasmiddelen door alcohol ethoxylaten, (2) de vervanging van zinken dakgoten door PVC-dakgoten, en (3) de vervanging van de brandvertragende stof HBCDD in isolatiemateriaal door twee alternatieve brandvertragers.

Trefwoorden:
Milieu effect analyse, chemische stoffen, socio-economische analyse, restrictie, autorisatie, REACH

Contents

Summary

In 2007, the European REACH legislation (Registration, Evaluation, Authorisation and restriction of Chemicals) came into force. The REACH legislation introduced the Socio-Economic Analysis (SEA) as a decision supporting instrument for authorisation requests or restriction proposals of hazardous chemical substances. In an SEA, the socio-economic costs of, for example, a restriction proposal are compared to the benefits of the restriction in terms of the reduction of impact on human health and/or the environment. As SEA is relatively new in the field of chemicals, there is a need for methodology development.

The goal of this report was to develop a versatile, scientifically sound, transparent and relatively simple methodological framework to quantify and compare expected environmental effects caused by chemical compounds. This should provide information on the relative environmental benefits if a hazardous substance would be replaced by a less harmful alternative, as input for an SEA. The methodology will make use of readily available methods and models. By developing this methodology, the RIVM contributes to reaching the goal of the Netherlands' Ministry of Infrastructure to be involved upfront in the SEA development process for the context of REACH.

The environmental impact assessment methodology described in this report consists of five consecutive steps: (1) scope and scenario definition, (2) exposure and hazard estimation, (3) determination of endpoints and assessment method, (4) environmental impact assessment, (5) dealing with uncertainties and (6) comparison of the scenarios and providing comparable information on environmental impacts.

(Step 1) In the scope and scenario definition, e.g., a minimum of two different scenarios is defined. For example, in case of a restriction, the Business As Usual scenario (BAU) representing the situation in which no policy action is taken and a Policy Scenario (PS) representing the situation in which a restriction is introduced. Further steps of the methodology will be performed for both scenarios.
(Step 2) The exposure and hazard estimation are comparable to what is generally done in risk assessment, except from the fact that in impact assessment we strive for realistic estimates instead of (realistic) worst case estimates.
(Step 3) The determination of endpoints and assessment methods is done on the basis of the data availability, the substances characteristics and the proportionality of the assessment in terms of required inputs and obtained outputs to come to conclusive results.
(Step 4) The assessment of environmental impacts of compounds involves the possibility of a ranking of PBT characteristics of substances and impact assessment based on a deterministic or probabilistic approach.
(Step 5) For the uncertainty assessment a standard table was developed which can be used to identify and document the main sources of uncertainty, providing a good comparison between BAU and PS including relative uncertainties.
(Step 6) Finally, an overall comparison of relative impact scores of both scenarios is made, using the acquired information from the previous steps.

The methodology developed in this report uses a tiered approach. This approach helps to choose the quality or level of detail of the assessment on the basis of data availability and the appropriateness of input compared to the (minimum) required output in order to come to conclusive results. In applying the methodology, one can start at a lower tier, moving to a higher tier whenever this is necessary to come to conclusive results and possible in terms of data availability. It is noted that for the results to be of use in the broader context of the socio-economic analysis, in general a higher tier will be required.

The methodology has been tested using three case studies of three different substances and their alternatives in a specific application. The case studies represent a range in possible hazard, fate, environmental impacts, data availability and uncertainty characteristics that can occur in practice: (1) the replacement of nonylphenol and nonylphenol ethoxylates (surfactant) in detergents by alcohol ethoxylates, (2) the replacement of zinc gutters by PVC (poly vinyl chloride) gutters, and (3) the replacement of the fire retardant HBCDD in insulating building material by two alternative flame retardants.

The methodology provides a relatively simple framework and practical guidance to estimate the environmental benefits of policy measures. With this methodology, the gap between risk estimates and impact estimate is bridged to achieve comparable impact scores. Developing and testing the methodological framework increased our understanding of the possibilities and impossibilities on environmental impact assessment and showed the major problems regarding, for example, data availability, uncertainty and the actual meaning (or practical value) of the end results. The exercise showed that it is possible, even with a limited amount of data, to move from risk indicators to impact indicators that are more useful in the context of the socio-economic analysis. It showed the importance of a robust uncertainty analysis in an assessment where a variety of input data, models and methods are used and connected, to understand the actual meaning of the end results. The case studies showed that the proposed methodology was feasible for the variety of the three tested cases, suggesting its applicability to a wide range of dossiers.

To further test the practical value of the environmental impact estimates produced by this methodology to SEA, further expansion of the scope towards other impact categories (socio-economic costs, human health, etc.) and valuation methods is required. This is one of the suggested follow-up activities presented in the report.

1 Introduction

1.1 REACH, risk assessment and socio-economic analysis

The European REACH regulation (Registration, Evaluation, Authorisation and restriction of CHemicals) came into force in June 2007 (EC, 2006). Two of the main goals of this regulation are:

- Improve the protection of human health and the environment from chemicals
- Enhance innovation and competitiveness of the EU Chemical industry

The REACH regulation has introduced socio-economic analysis (SEA) as a tool to support the decision making on authorisation requests or restriction proposals of substances in specific application(s). Both authorisation and restrictions are instruments of governments within the European Union to protect human health and the environment from hazardous substances:

- Authorisation involves the listing of a hazardous substance on Annex XIV of REACH. If a substance is listed on Annex XIV, companies who wish to continue the use of the substance, need to apply for an authorisation. Authorisations can be provided if risks to human health or the environment are adequately controlled or if the company shows that socio-economic benefits outweigh the risks to human health or the environment.
- Restrictions imply the setting of conditions on manufacturing, placing on the market or use of a substance (in a specific application) when the risk to the human health or the environment is unacceptable (REACH legal text articles 60 and 68).

An SEA helps to get an idea on the socio-economic impacts of a policy measure (a request for authorisation or a restriction) compared to the situation in which no policy measure is taken. The inclusion of an SEA is not mandatory for restriction proposals, while it can be mandatory in the case of an application for authorisation depending on the pathway of the authorisation procedure chosen (REACH legal text). In practice a more or less detailed SEA - showing the positive and negative impacts of a policy measure - can be very helpful in decision making on authorisation or restriction of chemicals. Recently, the first five SEAs were developed as part of the decision making on restrictions on five chemicals (Mercury, ECHA, 2010; DMFu, French competent authority, 2010a; lead and its compounds, French competent authority, 2010b; Phenylmercury compounds, Norwegian climate and pollution agency, 2010; Phthalates, Denmark, 2011).

As SEA is prescribed but rather new in the domain of chemical policy, ECHA published a Guidance on socio-economic analysis for restriction dossiers in 2008 and a Guidance on socio-economic analysis for the authorisation process in 2011 (ECHA 2008; ECHA 2011). These guidances provide a structure for producing and interpreting an SEA. Figure 1 gives an impression of the general structure of a socio-economic analysis.

Currently, the aforementioned guidances still leave many aspects of SEA open for interpretation. Further (methodological) development and testing of parts of SEA is desirable to improve the quality and usefulness of the SEA approach in the policy practices arising from Annex XV dossiers.

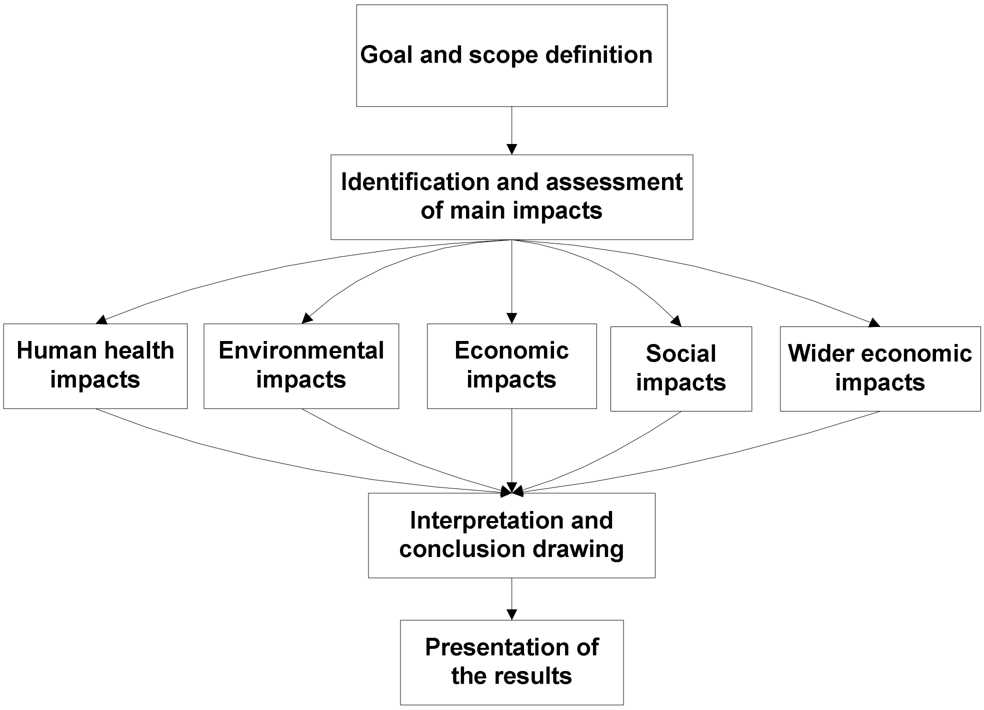

Figure 1: General SEA structure developed based on ECHA guidance (ECHA, 2008a)

1.2 Developing Socio-economic analysis methods

One part of SEA that requires further guidance is the qualitative and - if possible - quantitative description of the human health and environmental impact of the marketing, use and disposal of a substance and possible alternatives of that substance.

Current risk assessment practices give an indication of the risks coupled to the use of a chemical, summarized commonly by risk ratios (Risk Characterization Ratios, RCRs), i.e., the ratio of (predicted) ambient concentrations and a regulatory criterion concentration. RCRs for different cases are, however, often not comparable by nature. Each RCR > 1 indicates that there is a risk higher than the adopted limit value, but an RCR of 3 for substance X is not necessarily better than an RCR of 6 for substance Y, since the effect parameters on which the ratios are based often differ by nature and severity (e.g., thyroid atrophy versus liver tumours, mortality in aquatic organisms versus reproductive failure in predators) and as exposure and hazard estimates include (different) uncertainties. The incomparability of RCRs is a problem in the context of a socio-economic analysis, since one cannot thereby rank different Policy Scenarios to conclude what is the best in terms of minimizing impact on human or ecosystem health. For SEA, there is a need to adopt an impact assessment approach in addition to the RCR approach (which triggered the SEA). In this report building on to the existing SEA guidances, an environmental impact assessment methodology is presented which bridges the gap between risk assessment and impact assessment, and which allows for better comparison of the possible environmental impacts of Policy Scenarios.

This report focuses on the methodology development for environmental impact assessment of chemical substances. The report takes restrictions as the starting point as first experiences have been acquired in this field. The developed methodology, however, should also be useful for the authorisation process. Further development of human health impact assessment methodology is also relevant, but has not been dealt with in this report. However, the set-up of the proposed methodology is such that expansion with other impact modules (such as human health) is possible. For the latter, reference is made to the RIVM report on this SEA element (Schuur et al., 2008).

1.3 Summary problem definition

SEA and environmental impact assessment are both relatively new to the field of chemical substances regulation. In the current practice of restriction dossiers, the assessment of environmental impacts of the substances under consideration turns out to be complicated. Regular risk assessment results for chemicals, like RCRs, cannot directly be converted into environmental impact(s), and limited data availability and uncertainties are major drawbacks.

Thus, for SEA within REACH Annex XV authorisation and restriction dossiers, there is a need for the development of a scientifically sound, reproducible, transparent and generally accepted methodology for environmental impact assessment of chemicals. The methodology should enable one to compare environmental impacts caused by the use of different chemicals used for the same application (comparison of alternative scenarios). It should be as simple as possible and it should be applicable within the data constraints of the REACH regulation.

1.4 Goals and central question

This project aims to develop a prototype of a quantitative methodology for comparative environmental impact assessment of chemical substances. The project does not strive for the perfect methodology, but for a prototype of a methodology that can be further tested and strengthened in the practice of EIA and SEA of chemicals within REACH.

The central question of this report is:
What versatile, scientifically sound, reproducible, transparent and relatively simple methodology for quantitative environmental impact assessment of chemical substances can be developed for the comparison of environmental impacts of different substances used for the same purpose (scenarios)?

The methodology is versatile in the sense that it needs to deal with uncertainties and limited data availability and with straightforward as well as more complex risks and impacts. The methodology needs to be scientifically sound, reproducible, transparent and simple, to increase the understanding and acceptability of the methodology. The methodology needs to be comparative, because the environmental impacts of different scenarios for the use of chemicals for a specific application need to be compared by estimating the environmental improvement of shifting from one scenario to the other. Lastly, the methodology needs to be practicable to be useful in the practice of developing the environmental impact part of annex XV dossiers.

Within RIVM, expertise and knowledge on methods that can be useful in the environmental impact assessment of chemicals is available. We are thus convinced that by combining different expertises, we have at our disposal the basic ingredients that can help develop the methodology for environmental impact assessment of chemicals within the context of REACH. By exploring this field, the RIVM contributes to reaching the goal of the Netherlands' Ministry of Infrastructure and the Environment, namely to be involved upfront in the SEA development process that takes place at this moment in the context of the Socio-Economic Analysis Committee of ECHA in Helsinki. In more general terms, the goal of this project is to contribute to the development of SEA within REACH annex XV dossiers.

1.5 Scope and limitations

The project goal stated above is still very broad. The methodology that is developed should, in theory, include a wide variety of substances, hazardous effects, exposure routes to various environmental compartments and receptors (species, taxonomic groups, ecosystems, ecosystem functions). This would lead to a variety of environmental/ecological impacts at various geographical and temporal scales investigated at a specific level of certainty, based on (limited) data available. A broad scope runs the risk of loosening the focus during the development and testing of the methodology. Therefore, the scope of the project is limited on different aspects.

At first, the methodology is based on existing expertise, methods, data and models. The methodology is developed and tested using three case studies of three different substances and their alternatives in a specific application. The choice of the case study substances and their alternatives was specifically meant to include ranges in hazard, fate, environmental impacts, data availability and uncertainty that can occur in practice. Besides choosing three chemicals and their applications, choices on the geographical and temporal scale were needed to apply the methodology. This was done for each case study separately, taking the European context as a starting point. The chosen geographical and temporal scope can sometimes also be determined by the models used in various steps of the methodology.

This project focuses on the environmental impacts of chemicals including impacts caused by ecotoxicity, persistence and bioaccumulation of chemicals. Ecotoxicity includes a wide range of possible hazardous effects caused by the exposure of the environment to chemicals. This includes, among others endocrine disrupting effects. Effects can be acute or can appear in the longer run. Concerns about persistent, bioaccumulative and toxic substances (so-called PBT substances) are based on their potential to cause impacts on a large scale with regard to geography and time. Effects will typically occur over several generations. Besides, concerns were increased by the assumption that current risk assessment would not reflect the complex behaviour of the substances over their long life time. (Rorije et al., 2011). In principle, a 'safe' concentration for PBT (and vPvB) substances in the environment cannot be established with a sufficient reliability. Persistent and bioaccumulative properties allow substances to accumulate in remote environments, which is a process difficult to reverse, as cessation of emission will not immediately result in a reduction in chemical concentration due to the long half-life. In such cases, the target compartment and species at risk cannot be identified with sufficient accuracy, due to the long-term presence in the environment, secondary poisoning and extreme toxicity.

The focus on ecotoxicity has been chosen, because these hazard characteristics of substances are often the driver in the REACH restriction and authorisation process, when it comes to protecting the environment. Other environmental impact categories, such as climate change, resource depletion, acidification, etc. (as defined, in, among others, the life cycle assessment methodology – Goedkoop et al., 2009) will not be reviewed in the developed methodology. Other environmental impact categories might, however, be relevant as ‘background’ impact categories in specific cases. This happens, for example, if a substance in a specific application is not replaced by another chemical but by a completely different product or technique. Human health impacts (due to, e.g., carcinogenity, mutagenicity and reprotoxicity) are not included in this project. These impacts, however, are also relevant when it comes to the impact for REACH restrictions and authorisations. The processes followed in the impact assessment methodology are built in such a way that human health and other environmental impact categories can be added at a later stage. Economic valuation of the environmental impacts is required for SEA, however, this will not be included. Expansion of the project’s scope including valuation is possible at a later stage.

1.6 Reader’s guide

After this introduction, this report continues with an overview of the context of REACH, earlier work on SEA and environmental impact assessment in this context and an overview of what this report tries to contribute to that in chapter 2. Following that, the environmental impact assessment methodology is introduced in chapter 3. This chapter gives an explanation of the various steps of which the methodology consists. In chapter 4, the three case studies are introduced and an overview is given of what was actually done in- and resulted from - the case studies applying the methodology, the problems and discussion points that were confronted and the lessons learned. The report ends with a discussion chapter evaluating the work done, lessons learned and suggestions for further development and research. The report contains four appendices. Appendix A gives a proposal for practical guidance of the methodology for actual application. Appendices B, C and D give the full description of the case studies on respectively nonylphenol and nonylphenolethoxylates (NP/NPE) in detergent applications, zinc gutter systems and hexabromocyclododecane (HBCDD) in expanded polystyrene (EPS). The case studies were not meant to be fully comprehensive (i.e., ready to play a role in SEA). Rather, they were primarily carried out to enable learning in the process of developing SEA methodologies.

2 Literature review on EIA in SEA

In addition to the guidances published by ECHA on the socio-economic analysis as presented in the introduction (ECHA 2008, ECHA 2011), various reports have recently been published that contribute to the environmental impact assessment of substances in the context of REACH. These publications and their key-findings are discussed in this chapter.

2.1 State of the art theory and practice EIA in SEA

RPA report, 2010. Assessing the health and environmental impacts in the context of socio-economic analysis under REACH.

The logical framework described in this report has been designed to be consistent with the ECHA Guidance on preparing SEAs for Restriction and Authorisation. The five main steps in the logical framework for assessing health and environmental impacts can be summarized as follows:

- **Step 1: Characterization and scoping assessment** – using the available data to define the scope of the impact assessment to be carried out (linked to Stage 2 of the ECHA guidance).
- **Step 2: Qualitative to semi-quantitative assessment of impacts** – drawing data from the chemical safety assessment and other sources to provide a detailed description of potential impacts (Stage 3 in the ECHA guidance).
- **Step 3: Quantitative assessment of exposures and impact** – where feasible and appropriate, developing further quantitative data to support decision making. This may take place on two levels: comparison against benchmarks, or predictions of changes in the population or stock at risk; and quantification of the associated changes in impacts on that population or environmental stock.
- **Step 4: Valuation of impacts** – estimating the economic value of the change in impacts using methods and units of measure appropriate to health or the environment (e.g., willingness to pay values, health care costs, market value of changes in productivity, etc.).
- **Step 5**: **Comparative analysis –** analysing the changes in health or environmental effects and determining whether the net change is positive or negative.

With regard to the environmental impact assessment, the methodology is a stepwise approach in accordance with the approach proposed in this report. The RPA report discusses various approaches towards both qualitative and quantitative assessment of impacts in more detail. Quantitative approaches presented are:

- Use of simple physical indicators as proxies for impact, for example, tonnage used, number of sites emitting a substance into the environment, quantity of the substance emitted to the environment or data on monitored levels in the environment.
- Use of dose-response data or SSDs models to provide information on the potential impacts on sensitive species, or
- Fuller quantification of environmental impacts by combining dose-response, SSDs or systems level data with measured or modelled

(distributions of) environmental concentration data to predict the impacts on different ecosystems or food chains.

Key findings were:

1. The process relies on collation of a range of information from existing sources such as the REACH Chemical Safety Assessment and associated exposure scenarios; however, it also demands additional information in order to produce robust information for use by decision makers.
2. The extent to which the above types of information will be available is likely to vary. For example, production and use pattern information – together with information on site locations – may be readily available from REACH Registration dossiers to authorities preparing restriction SEAs, or to an industry consortium; it will be harder for a downstream user to use them within the wider EU context, but some of this information may be available from ECHA Annex XV dossiers.
3. The development of robust and comprehensive qualitative and/or quantitative assessments of health or environmental impacts requires a multidisciplinary approach involving a multidisciplinary team of experts.
4. Among a long list of recommendations for further research, key recommendations are the interpretation of ecotoxic effects in relation to environmental impacts, further development of Life Cycle Impact Assessment models, in order to be more consistent with concepts and methods under REACH and the development of more hazardous chemicals relevant ecosystem services concepts. An issue for special attention is the evaluation of chemicals that are very persistent and very bioaccumulative but for which no particular toxicological concerns have yet been identified (i.e., vPvB). For such substances, even if information on geographical and temporal patterns of exposure can be derived, there is no suitable metric of effect (i.e., toxicity to particular organism(s)) against which to establish an impact valuation. With regard to exposure estimation, one of the recommendations is to better define the limitations and uncertainties surrounding the various models and approaches. In respect of both the effects of substances and the estimation of exposure, further research may establish the added value gained by adopting a probabilistic (non-deterministic) approach when estimating exposures and then linking these to effects.
5. The ‘ecosystem services’ approach is recognized as a powerful tool for establishing the potential socio-economic importance of the goods and services provided by the environment that may be at risk under the alternative chemical use scenarios. However, it is not necessarily easy for those unfamiliar with the concept to make linkages between the types of impacts that hazardous chemicals can have on the environment and the outputs from risk assessments.

WCA-Environment, 2011. Refinement of environmental risk assessment outputs for use in socio-economic impact assessment under REACH.

This report tests the utility of ‘relatively simple and rapid approaches’ for the translation of ecological risk assessment output into impacts for SEA: LCA, SSD, exposure based proxies and read across methods from similar substances. Four substances and their potential substitutes were selected for detailed case studies (1,2,4 trichlorbenzene and (mono)chlorobenzene; chloroform and dichloromethane; nonylphenol and alcohol ethoxylates; short-chain chlorinated paraffins). In addition, the more complex ecosystem services approach was tested on one substance and its potential substitute.

The most important conclusions on the Life Cycle Impact Assessment (LCIA)/SSD method are:

1. Useful method to normalise environmental impact of chemical emissions and expression of this impact in terms of equivalents, such as volume of media affected (exposure-based proxy, generated by probabilistic EUSES modelling) or percentage of species affected (estimated ecological risk).
2. Data availability is a crucial, often limiting, factor. Filling data gaps with QSARs is likely to inconsistently describe the toxicity of a chemical and should be applied with caution. Another source of great uncertainty is caused by the application of equilibrium partitioning.
3. It is problematic to assess assumptions and limitations since methodologies and calculations underpinning the LCIA are not readily available.
4. The techniques that incorporate uncertainty are considered to be particularly relevant for a robust assessment of the difference in impacts of different risk management options, particularly those involving substitute chemicals with relatively poorly understood ecotoxicity.

With regard to the ecosystem services approach, it was concluded that this is a useful alternative tool for communication of the risk or impact, but offers no additional analytical benefit over conventional risk assessment. The technique identifies impacts using a causal chain, but offers no additional means to value the impact of a chemical on the particular service.

ECETOC, 2011. Environmental impact assessment for socio-economic analysis of chemicals: principles and practice. Technical Report No. 113.

This report reviews, without giving much detail, relevant existing principles and practices for SEA, among others with reference to the ECHA Guidance, and describes its requirements, among others with regard to data and valuation. The report argues for as much quantification of ecological impacts as possible with the ideal of monetisation in order to carry out a cost-benefit analysis. It is acknowledged that, currently, regulatory ecological risk assessments do not express effects in terms of quantitative impacts and proposes methods to do so such as an analysis based on SSDs, smart modelling (modelling of population densities and/or biomass in relation to exposure), making connections to ecological quality status (for instance those of the Water Framework Directive) and an ecosystem services approach. In addition, it is also noted that valuation of ecological impacts is problematic, especially for non-marketed ecological goods and services.

2.2 Key gaps and approaches addressed in this report

Wherever possible, this report on methodology development took into account the insights obtained by the studies described above. However, due to the timing of publication this was not always possible as projects have been performed in parallel. The methodology described in this report mostly has connections to the work of RPA and WCA environment.

Like the RPA report, this report takes a stepwise approach. The combination of steps is designed in such a way that a logic, fairly simple and understandable framework is created. The steps are explained in the main text of the report and are further worked out in terms of required actions per step to give assessors hands-on help in performing an environmental impact assessment for restriction or authorisation dossiers.

The basis of the methodology is the definition of (alternative) scenarios of chemicals use and emissions. This is the starting point of the environmental impact assessment of chemicals. This starting point can also be used as the basis for the estimation of other impact categories like human health, other (non-toxicity) environmental impact categories, market impacts, etc. Although the methodology worked out in this project takes a narrow scope by only looking at environmental impacts caused by ecotoxicity characteristics of chemicals, the methodology is built in such a way that expansion with additional impact (or economic valuation) modules is possible.

The methodology described in this project focuses on quantitative estimation of impacts, proposing three different methods to do so. The methodology takes a tiered approach in all major steps of the assessment, allowing for the selection of the appropriate manner and level of detail of the assessment based on what is possible with the data available and what is required to fulfil the goal of the assessment. A tiered approach includes a deterministic as well as a full probabilistic environmental impact assessment method based on probabilistic exposure estimates and species sensitivity distributions. The deterministic approach is based on the ecotoxicity module of ReCiPe Life Cycle assessment (LCA, Goedkoop et al., 2009). ReCiPe is an LCA model that was developed integrating various existing LCA models (CML LCA, Ecoindicator 99). The model was developed on the basis of consensus, initiated by a large number of LCA experts who expressed the desire to have a common framework for LCA. The ReCiPe model is now developing into the standard LCA method used in different (international) LCA studies. The basics of these two methods as used in this report are carefully described, in order to increase understanding and acceptability. The deterministic and probabilistic approaches are complementary in a tiered approach, but can also be used subsequently, as stand alone or in parallel. If used in parallel, the results can be compared to evaluate and better understand the impact estimates of the lower tier approach (in this case, the deterministic one). The third method is specially meant for substances with persistent, bioaccumulative and toxic characteristics. This method gives a quantitative estimate of P, B and T that can be evaluated next to other impact estimate(s) on ecotoxicity for secondary poisoning at least.

Lastly, the methodology developed addresses the fairly important role of uncertainty analysis as part of the overall impact assessment. The reason for this is that in this type of scenario-based assessments, using a wide range of input parameters and models, there will inherently be a wide variation in sources of uncertainties that might influence the end results. The diversity in possible sources of uncertainties and the lack of experience in dealing with them stimulated us to build a framework to deal with these uncertainties.

The mail general types of uncertainty should be mentioned at this early stage:

1. Data availability: the extent to which information will be available is likely to vary within scenarios as well as between scenarios.
2. Data quality: the reliability and validity of the information is also likely to vary. Filling data gaps with QSARs, for instance, might introduce additional uncertainty, if the QSAR model is used to extrapolate outside the known boundaries. Nevertheless, a QSAR prediction might also yield less

uncertainty in specific cases, when compared to experimental measurements that are variable because of high biological variability, or highly uncertain because of problematic analytical procedures for specific classes of substances.

3. The extent of the uncertainty caused by both data availability and quality may vary between the Business As Usual (BAU) scenario and the Policy Scenario (PS). It is likely that more data of known quality are available for the former than for the proposed alternative, which may make a comparison problematic.
4. This report will propose methods for dealing with both quantifiable and unquantifiable uncertainties. However, it should be recognised that some uncertainties are difficult to capture, e.g.*,* scenario and model uncertainty,
5. Availability of expert knowledge: the development of robust and comprehensive qualitative and/or quantitative assessments requires sufficient, multidisciplinary expertise to avoid black box approaches of the instruments available.

3 Methodology of environmental impact assessment of substances

3.1 Outline of the methodology

The figure below gives a schematic presentation of the environmental impact assessment methodology of substances as developed in this project. The methodology intends to give practical guidance on the quantification of the environmental impact of a specific policy measure (e.g., restriction or authorisation) for a chemical substance. The methodology is based on existing methods developed in the context of risk assessment and environmental impact assessment. In the sections below, the various steps of the methodology are explained. A full practical guidance to apply the methodology is given in Appendix A.

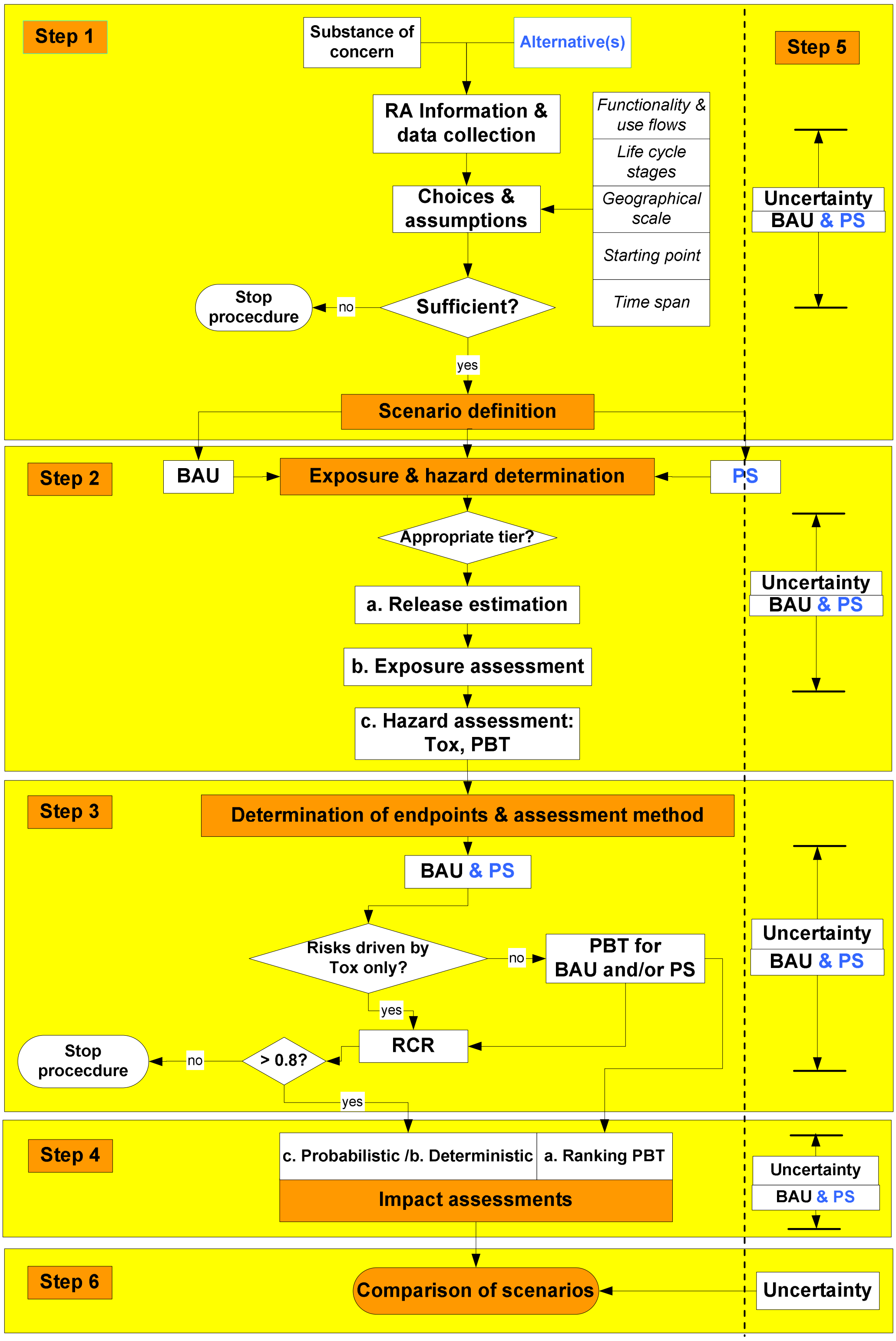

Figure 2: Schematic presentation of the methodology
RA = Risk Assessment; BAU = Business As Usual scenario; PS = Policy Scenario;
Tox = Ecotoxicity; PBT = Persistent, Bioaccumulative and Toxic

3.2 Step 1: Scope and scenario definition

3.2.1 Description

The EIA process starts with a substance of concern for which a policy measure is considered and the identification of possible alternatives of the substance of concern. The application of the methodology should result in a description of the environmental impact of a policy measure on a substance like a restriction or authorisation. In this report 'restriction' is taken as the starting point for scenario development. In an EIA, a comparison is made of the environmental impact of the scenario on what would happen if no policy measure were implemented, i.e., the Business As Usual (BAU, continued use of substance of concern), and the environmental impact of the Policy Scenario(s) (PS) representing the situation if manufacturing, placing on the market and/or usage of substance X in application Y is restricted and the substance of concern is thus replaced by (an) alternative(s).

The first step of the methodology consists of the scope and scenario definition. This includes the first data collection and the making of choices and assumptions on a variety of aspects. Table 1 below gives a general overview of the activities and explanation of this first step.

3.2.2 Sufficient to continue?

The effort put into the development of an EIA should be proportional to the goal it serves. It is therefore very important to consider early on in the process whether it is *possible* and *relevant* for the case under study to perform an EIA. The consideration of the proportionality of the assessment will be further refined in the next steps of the methodology by taking a tiered approach, to consciously choose the appropriate level of detail of every step in the assessment.

- Whether it is *possible* to do an environmental impact assessment depends on the data availability. If not enough data are available, for example, on possible alternatives, exposure and hazard characteristics, it might not be possible to complete the impact assessment. It was not possible to define absolute minimum data requirements for the substance of concern and its alternatives as this can be seen to be case-specific. However, as the reason to start this assessment is a concern about the hazardousness of a substance, it is assumed that a minimum set of data will always be available for the substance of concern. Alternatively, the availability of data will in general be more problematic, as there has not necessarily been an incentive to produce toxicity data for this substance. In many cases, this can be solved by taking (worst-case) assumptions, resulting in higher uncertainties for the PS. However, if data availability is very limited, one could also decide to collect more data, e.g., to urge industry or other stakeholders to provide more data. This might imply a (temporary) stop of the impact assessment process.
- Whether it is relevant to perform an EIA of the substance of concern and its alternative(s) depends on whether or not the substance of concern and the alternative substance(s) are expected to cause harmful effects to the environment (reviewing all environmental compartments including secondary poisoning) based on the available knowledge. When no harmful effects are expected, there is no need to perform an environmental impact assessment. Note that the conclusion that no ecotoxic environmental effects

are expected does not necessarily mean that the substances under study are not harmful, as they might affect, e.g., human health.

Table 1: Overview of the activities and explanation of step 1

Activities	Explanation
First data collection	General data and toxicity data on substance of concern and possible alternatives
Investigate substance of concern, application(s) and alternatives	Amounts, hazards, environmental compartments, RCRs if readily available
Decide whether EIA is possible and relevant	Based on data availability and indication of environmental concern
Choices and assumptions	substance, application, alternatives replacement ratio included life cycle stages, such as the waste stage geographical scale (of the restriction and of the impact) starting point in time of policy measure time frame reviewed in the assessment (of restriction and of the impact) critical toxic effects and environmental compartments of concern
Define BAU	Production, use, import, export amounts, expected market trends
Define PS	The actual restriction (production, placing on the market, use), expected reduction, replacement alternative

3.3 Step 2: Exposure and hazard assessment

The second step of the methodology follows the logic of the standard risk assessment methodology including the release estimation, exposure and hazard assessment.

3.3.1 Tiered approach

The exposure and dose-effect or hazard assessment can be done at various levels of detail/qualities. Exposure estimates can be expressed in terms of, e.g., point estimates or probabilistic exposure distributions using a variety of possible data sources. Dose-response estimates can be expressed in terms of, e.g., single species acute or chronic estimates or species sensitivity distribution, again using a variety of possible data sources. The two ‘extremes’ are presented below, but in practice middle cases will often occur.

- *Minimum quality* includes: release estimation based on Emission Scenario Documents (ESDs), Emission Release Categories (ERCs) or Sector specific Environmental Release Categories (SpERCs); point exposure estimation(s) by applying the European Union Systems for the Evaluation of Substances (EUSES); (dose-)effect data for water and a limited number of species or some hazard data derived from QSAR models. This assessment in general will have a low accuracy. Uncertainties will be largely unknown and therefore difficult to quantify, and because of this a conservative or more protective approach is appropriate.

- *Preferred* or *'maximum' quality* includes*:* release estimation (partly) based on actual measurements including uncertainties; exposure assessment in EUSES based on real data, optionally including probabilistic estimation of the exposure; (dose-)effect data for all environmental compartments, and sufficient number of species to determine the species sensitivity distribution function (SSD) for each environmental compartment, derived from experimental studies and checked by QSAR models (by the Weight of Evidence method). This assessment has a higher accuracy, uncertainties in general can be described quantitatively (probabilistic), and the assessment can therefore be more realistic.

The different levels of detail or quality as described above, introduce a so-called 'tiered' approach to the EIA-assessment. The minimum quality represents the lowest tier (like tier 1 in Figure 3) and the preferred quality represents the higher tier (like tier 4 in Figure 3). Between the minimum and 'maximum' tier, there is, of course, a broad range of intermediate tiers both in terms of the exposure and of the effect assessment. Whether to perform the assessment at minimum or preferred quality depends on the data availability of BAU and PS and on the proportionate or required level of detail to come to conclusive results. The principles and implications of the tiered approach are illustrated in Figure 3 below: tiering in risk and impact assessment allows one to optimize between practical aspects of the EIA (cost-efficiency, proportionality, time expenditure, etc.) and scientific needs (specificity, appropriate model given the problem definition, etc.). At this moment in time, one will not always be able to estimate what tier is proportionate. Therefore, it might be necessary to come back to the choice made here and to further refine the analysis done. One can thus apply the tiered approach in a dynamic way, starting at a low tier, and stepping up a tier whenever necessary and possible to come to conclusive results. In general, one could say that a higher tier is chosen in case the difference between BAU and PS is less obvious while still considered important, e.g., environmentally or regarding costs of the alternative scenario. A higher tier is also required when the end results are to be used as input for a wider socio-economic assessment as this will result in more realistic impact estimates.
The tiered approach had been introduced earlier by Solomon et al. (2008) in the context of ecotoxicological effect characterization of chemicals.

Table 2 gives an overview of the outputs of step 2 at various levels of quality.

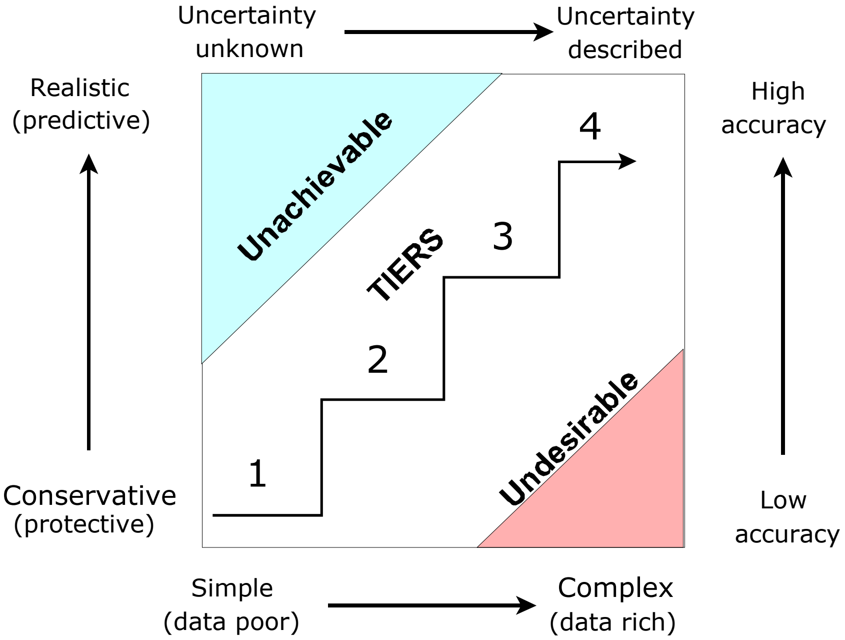

Figure 3: The tiered approach to link risk and impact assessments, with its practical and scientific consequences (Solomon et al. 2008)

3.3.2 Step 2a: Release estimation for the Business As Usual- and Policy Scenario

As mentioned above, release information can be based on measured release data or on model based release estimates, i.e., release quantities or release factors. Preferably releases into the environment should be based on measured data (although these also have drawbacks as number of measurements, measuring method, etc. might not be sufficient). If there are no measured data available, releases will have to be determined by applying release estimation methods. These can be engineering calculations or estimation methods usually containing typical release factors described in ESDs, ERCs or SpERCs (for further explanation, see the textbox below).

The ESDs or SpERCs can be used in the quantification of emissions to air, water and soil. The relevant emission assessment approach for the substance of concern and the alternative need to be chosen. When a substance and the alternative are compared for a specific application, the same ESD is generally applicable to both the substance of concern and the alternative. Possibly, another ESD has to be used in case of a different functional description of the use of the alternative.

Textbox: Explanation of release estimation in ESD and SpERC
Basically, an ESD describes the sources, production process, pathways and use patterns with the aim of quantifying the emission (or release) of a chemical into water, air, soil and/or solid waste. An ESD ideally includes all the following life cycle stages: (1) production, (2) formulation, (3) industrial use, (4) professional use, (5) private and consumer use, (6) service life of product/article, (7) recovery, and (8) waste disposal (incineration, landfill). In general, the ESD focuses on the use of a substance. The life cycle stages following on use, service life of a product/article containing the substance and waste treatment (paper recycling, landfill) are not always covered by an ESD. When ESDs are used in environmental impact assessment, one should therefore be very attentive to which life cycle stages are included and which are not, and state this explicitly in the assessment report.
In the context of REACH, the industry started to develop Sector sPecific Environmental Release Categories (SpERC). Many of these SpERCs are based on available ESDs. In addition industry generated additional data for those industry sectors not yet covered by the already available ESDs.

3.3.3 *Step 2b. Exposure assessment for the Business As Usual- and Policy Scenario*

After estimating the releases into the environment, the substance concentrations the various environmental compartments can be calculated using fate and distribution models. For this purpose, either the EUSES model, developed by the European Commission, or the ECETOC TRA model can be applied. Both models are based on two fate models: SIMPLEBOX and SIMPLETREAT. The EUSES model contains default environment settings for the local (around point source), regional (country) and continental (EU) scale and a sewage treatment module for each of these scales. The ECETOC TRA model is a spread sheet version of the EUSES model. To be able to use exposure models for the calculation of Predicted Environmental Concentrations (PECs), in addition to the release fractions from step 2a, information is required on physical chemical properties, biodegradability and chemical class.

3.3.4 *Step 2c. Hazard assessment for the Business As Usual- and Policy Scenario*

In environmental risk assessment, the potential harmful effect (or risk) can be derived by dividing a predicted environmental concentration (PEC, derived in step 2b) by a predicted no-effect concentration (PNEC) representing the hazard (dose-effect) characteristics of the substances. The hazard characteristics of the substances are based on standard laboratory toxicity test data. The minimum set of toxicity data needed depends on the endpoints to be assessed. The current methodology focuses on the primary environmental compartments and the sewage treatment plant. Secondary poisoning might (or should) be included if relevant, for example, if substances under study are indicated to have PBT characteristics. Man indirectly exposed via the environment is not included in this project.
The PNEC for water and soil organisms can only be determined on the basis of acute toxicity test results from each of the three trophic levels of the base set (fish, daphnia, algae) by applying assessment factors. Assessment factors depend on various issues. Lower assessment factors are applied when a higher number of different trophic levels are covered in the data set, and when the

duration of the toxicity tests is chronic. It is expected that, for the substances of concern at least, acute or chronic toxicity data for four taxonomical groups will be available, as the concern on the substance will generally be based on a number of prescribed hazard tests. For the alternative substance(s), data availability will be generally lower. When hazard data are very limited, one could try to produce more toxicity data by using Quantitative Structure-Activity Relationship (QSAR), or Ecological Structure Activity Relationship (ECOSAR) models (EPISuite 4.0, 2009). These models can also be used in case of high data availability, in addition to experimental data to reduce data uncertainty (using a Weight of Evidence approach).
When there are no data on sediment or soil organisms, the PNEC can be calculated from aquatic PNEC by using the equilibrium partitioning method. For the sewage treatment, plant toxicity data for micro-organisms in the Sewage Treatment Plant (STP) have to be provided. Usually, growth or respiration inhibition tests providing a NOEC, EC10 or EC50 are used for this purpose.

Table 2: Overview of the outputs of step 2 at different levels of quality

Step 2	**Minimum quality** (‘tier 1’)	**Preferred quality** (‘tier 4’)
a. Release estimation	Release factors to air, water and/or soil for one or more life cycle stages based on ESD/ERC/SpERC	Release factors to air, water and soil for all relevant life cycle stages based on actual emissions and modelling results, including indication of uncertainties
b. Exposure estimation	PECs calculated on the basis of point estimates using EUSES, no quantitative uncertainty indicators	PECs calculated (partly) on the basis of actual measurements using EUSES, quantitative uncertainty indicators (distributions)
c. Hazard assessment	PNECs based on fish, daphnia and algae acute toxicity tests, for all available environmental compartments, if necessary/possible complemented with QSAR/ECOSAR estimates	PNECs based on more than three taxonomic groups using acute and chronic toxicity tests, for all relevant environmental compartments, checked by QSAR estimates

3.4 Step 3: Determination of endpoints and assessment methods

In this step, the endpoints and environmental impact assessment methods for the case under study are chosen and a decision whether or not the impact assessment is useful is made, following the decision scheme of the methodology shown in Figure 2. Before we start performing a risk characterization and environmental impact assessment of the BAU and PS, it is important to consider the issues treated below.

3.4.1 Choice of assessment method

This methodology includes three different impact assessment methods:

a. PBT ranking,
b. deterministic impact assessment and
c. probabilistic impact assessment.

The PBT ranking method is meant for PBT (PBT like or vPvB substances) and will be used along with one of the other impact assessment methods. The deterministic and probabilistic methods are basically comparable but they differ in, e.g., input requirements and accuracy of the results, i.e., they are subsequent tiers. The results of the deterministic approach will generally be more conservative, especially when predefined conservative data, approaches and models are applied. The results of the probabilistic approach will be more realistic, especially when all aspects are tailored to the problem (highly specific). Further explanation of the three steps is given in section 3.5. At this stage, the decision is made which method(s) is (are) most meaningful to estimate whether implementation of the restriction results in net environmental benefits (or costs).
Crucial aspects in the determination of the assessment method are:

1) the availability of data for both BAU and PS,
2) the relevant adverse ecotoxicity endpoints (toxicity, persistence, bioaccumulation), and
3) the proportionality of the assessment in terms of required inputs and obtained outputs to come to conclusive results.

1. The availability of data determines what assessment method *can* be applied: PBT ranking, deterministic and/or probabilistic impact assessment. Overall, the deterministic approach requires fewer input data than the probabilistic approach. Note that the deterministic and probabilistic approaches are two extremes, when both exposure and effect assessment are fully probabilistic or not. If enough data are available to produce an SSD (three or four toxicity studies, usually for at least three different taxonomic groups[1]; probabilistic effect assessment), but there are not enough data to derive probabilistic exposure estimates (or the other way around), one could use a ‘semi-probabilistic’ approach using point exposure estimates instead of probability exposure distributions (further explained in step 4c) in combination with SSD-modelling.
To make sure the end results will be comparable, the same impact assessment methods should be used for both BAU and PS. The available data for the PS are expected to be considerably fewer in number than those for the BAU. In that

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[1] Note that a (very) tailored approach with SSD modeling could imply the fitting of an SSD to a selected subset of typical species data, tailored to the expected environmental problem. This can be explained by means of an example of a highly specific Toxic Mode of Action. When in such a case scenarios would be compared, it might be appropriate to derive an SSD for both target organisms (insects) and non-targets organisms (side effects). See Posthuma et al. (2002) Chapter 22.

case, the data availability of the PS will determine the level of detail of the assessment.

2. Relevant adverse ecotoxicity endpoints can easily be determined on the basis of the hazard data (step 2c) for both scenarios.

- When adverse environmental effects of both BAU and PS are driven by toxicity only (and not by persistence and bioaccumulation potential; T and not P and B), either the deterministic (b) or the probabilistic (c) impact assessment method will be applied.
- When adverse environmental effects of *one of the substances* in BAU or PS, are (or might be) driven by persistence, bioaccumulation and toxicity, the PBT ranking method will be applied. Impact assessment will be very difficult (or even impossible) for PBT substances, because of the long life-time and difficulties in determining accurate exposures for these substances. Nevertheless, we decided to perform the probabilistic impact assessment method for PBT substances, to get an impression of the expected releases (and exposure) in combination with the toxicity. This impact assessment should *at least* include *secondary poisoning* as environmental 'compartment', as the concern of PBT substances is related to bioaccumulation and biomagnification. Note that the deterministic impact assessment method is not included here, as secondary poisoning is not included in the standard modules used in this method.

3. What level of detail of the assessment is proportional depends on what accuracy is required to come to decisive results. As mentioned earlier, one could say in general that in cases where the difference between the impact results of BAU and PS is rather obvious, a lower tier approach can be applied (deterministic approach). A higher tier approach (probabilistic approach) is chosen in cases where differences are less obvious. The 'semi'-probabilistic approach using point exposure estimates can be seen as an in-between tier. It should be mentioned that the higher tier approach is preferred when results are intended to be used as input for a wider socio-economic analysis, as this will provide more realistic end results.

Overall, the above consideration can result in the following methods to be applied:

- PBT ranking + probabilistic impact assessment at least for secondary poisoning
- Deterministic impact assessment
- Probabilistic impact assessment

for which the tiering is driven by the specific needs of the comparison, and the availability of data.

3.4.2 *Decision whether it is useful to perform an impact assessment*

The decision whether or not it is useful to perform an environmental impact assessment is made on the basis of the calculation of Risk Characterization Ratios (RCRs) for both the BAU and the PS for all relevant environmental compartments. RCRs give a first indication of the risk according to current policies, in which an RCR > 1 indicates a risk, and an RCR < 1 indicates that there is no risk beyond the (policy-chosen) criterion (PEC is lower than PNEC; measured or expected exposure is below a level considered safe).

- If RCRs of both BAU and PS are < 1 for all environmental compartments, this indicates that there is no risk and one could conclude that in this case, no impact (or impact difference) for BAU and PS is to be expected either. Strictly, an RCR below 1 could serve as cut-off criterion here. However, due to expected ranges in the data uncertainty and the related possible cases incorrectly surpassing the RCR of 1, an (arbitrary) RCR value of 0.8 is proposed as a pivot point on which to decide whether to go on or stop the EIA procedure. Hence, if RCR values below 0.8 are obtained for both scenarios the EIA will be stopped. Note that the cut-off RCR value of 0.8 is arbitrary chosen. We expect no impacts or only minor impacts below this RCR value and no significant impact difference between BAU and PS at such small risk indications. This expectation is derived from literature studies which looked at the question whether field species assemblages are affected at a PNEC-type field exposure level; in such studies, impacts were generally not found (see, e.g., Mebane 2011 for a recent review). However, the actual accurate cut-off RCR value below which in practice no environmental effect occurs could be determined at a better scientific foundation.

- If (all) the RCRs of BAU are > 0.8 and those of PS are < 0.8 (or the other way around) one could conclude that the one scenario is better (less risky) than the other, and purely to conclude what is the better scenario, one could stop the assessment here. However, as a RCR of 1 does not necessarily mean that there is an impact, and as one wants to get a more detailed estimation of the level of improvement for the broader context of the socio-economic analysis, we suggest to proceed with the analysis in this case as well, and to perform an appropriate impact assessment, starting at a lower EIA-tier.
- If RCRs of both BAU and PS are > 0.8, a difference in risk and impacts is not excluded with sufficient certainty, and impact is considered for both scenarios. To conclude what scenario is better in terms of impact, the analysis will be continued.

3.5 Step 4: Environmental impact assessment of chemical substances

3.5.1 Step 4a: PBT ranking

In principle, when the substance of concern or the alternative(s) is (are) identified as potential PBT or vPvB, the risk and impacts are difficult to quantify with accuracy. In these cases, the concern for persistence, bioaccumulation and toxicity of each substance are clear proxies for real concern. P, B and T scores will therefore be used as impact indicators for these substances. PBT-type scorings of the BAU and the PS scenarios will be compared on the basis of quantitative, continuous P, B and T scores, in accordance with the methodologies developed by Rorije et al. (2011), combined with the toxicity assessment presented here. If necessary, the Long Range Transport Potential (LRTP) of a substance can also be scored and added according to the equation provided by Rorije et al. (2011). To summarize a PBT score, the separate values obtained for P, B and T are summed.

The equations 1 and 2 to score for persistency and bioaccumulation are presented below. The method to centre, scale and transform the data to score for persistency and bioaccumulation is presented in section 2.2 of the RIVM report on identifying potential POP and PBT substances (Rorije et al., 2011). For further explanation of the equations, the reader is referred to the report of Rorije et al. (2011). In both formulae, the score is given in relation to a chosen reference P or B value (180 and 5000, see below).

$$P_{score} = e^{\frac{-\ln(2)*180}{P_{ov}}} \qquad \text{Eq.1}$$

In which:
Pov = Overall Persistence (days) calculated using the OECD Pov & LRTP Screening Tool and depends on the log Kow, log Koa and half-life in air, water and soil (Rorije et al., 2011).

$$B_{score} = e^{\frac{-\ln(2)*5000}{BAF}} \qquad \text{Eq.2}$$

In which:
BAF = the Bioaccumulation Factor for birds and mammals (secondary poisoning).

Rorije et al. (2011) did not provide a ranking equation for toxicity. To obtain a complete picture of the P, B as well as T, a scoring method for toxicity was added, using the same type of transformation function. Just as for the P and B score, the T score can be used to determine the likelihood that a substance fulfils the PBT-criterion. Therefore, it has been decided to centre on toxicity data around a PNEC of 1 µg/l for the aquatic compartment, based on the criterion of Annex XIII 10 µg/l divided by 10 as the standard assessment factor for chronic toxicity. This results in the following equation, where the PNEC has to be expressed in µg/l.

$$T_{score} = 1 - e^{\frac{-\ln(2)*1}{PNEC}} \qquad \text{Eq.3}$$

In which:
PNEC = the Predicted No-Effect Concentration.
Using this formula, the largest changes in T score will occur between a PNEC range of 0.1 and 10 µg/l.

To make the scorings of BAU and PS comparable, similar input data should be used when calculating the scores. Preferably, measured data should be used, however, the method provided by Rorije et al. (2011) is particularly developed to score data-poor substances based on QSAR estimates and is therefore also useful to allow for comparison between BAU and PS when experimental data on persistency and/or bioaccumulation are lacking.
For BAU and PS, the toxicity data set may not be equally available, and consequently not all substances can be equally weighed on the basis of the lowest chronic toxicity data point. The use of assessment factors to derive PNEC values is introduced to account for this. The PNECs derived in step 2 are used to obtain T scores instead of the lowest toxicity values. If, however, reliable QSAR models are available to predict missing chronic toxicity data, this could be used instead of assessment factors.

The scores for persistency, bioaccumulation and toxicity are summed to come to a total PBT score that will vary between 0 and 3, which – by virtue of the methods used – is a purely relative value that enables relative ranking of the BAU and the PS scenario.

Note that the PBT and vPvB criteria for Annex XIII to the Regulation do not apply to inorganic substances (ECHA, 2008b). The PBT ranking method cannot be applied to these substances. Depending on the number of inorganic alternatives included in a study, it might not be useful to perform a PBT ranking, as the ranking is a comparative method.

3.5.2 *Step 4b: Environmental impact assessment based on a deterministic approach*

This method is based on determining substance-specific characterization factors (CFs) which combine exposure and effect to represent the relative contribution of the substance to environmental impacts. Regarding background knowledge, the method is in part probabilistic, in the sense that the tabulated (or generated) data used can originate from probabilistic approaches. We refer to the method as deterministic here, since the method can be run by combining tabulated (fixed) data, which yields outputs for the two scenarios driven by pre-defined choices and underlying research. In the probabilistic method described below, the data and models chosen are specifically tailored to the problem, although the models strongly resemble the underlying models of the deterministic analysis.

CF consists of a fate factor, *F*, relating an increase of concentration to an increase of emission and an effect factor, *E*, which expresses the increment of effect or damage due to a marginal increase of the concentration:

$$CF_{i,j,s} = F_{i,j,s} \cdot E_{j,s} \qquad \text{Eq.4}$$

where $CF_{i,j,s}$ (year.kg^{-1}) is the compartment-specific environmental characterization factor of chemical *s* emitted to compartment *i* and transported to and degraded in compartment *j*. This characterization factor (*CF*) will finally be multiplied by the emission rate to compartment *j* to come to an impact score (fraction potentially disappeared species) of the chemical substance. The individual parts of the equation 4 will be further explained before coming to the final impact score formula.

The fate factor

The marginal change in the environmental dissolved steady state concentration due to a marginal emission change is defined as the ecological fate factor (Huijbregts et al., 2005a). The multimedia model USES-LCA (USES-LCA 2.0, consisting of the nested multimedia fate model Simplebox 2.0, developed by Brandes et al. (1996) and the newest version of EUSES (EC, 2004)) is used to determine the fate factor. Fate factors have been calculated for a large number of chemical substances, using the method described here, and they have been published by Huijbregts (2004). These published fate factors can be used in the calculation of the final impact score. Note that for each of the environmental compartments *i* (emitted) and *j* (transported) a number of fate factors may exist, in case the substance *s* is emitted to a number of different environmental compartments *i* and transported to different environmental compartments *j*. All relevant fate factors should be included in the final calculation.

The effect factor

The effect factor is based on the potentially disappeared fraction of species (PDF) which is the fraction of species that has a high probability of no occurrence in a region due to unfavourable conditions. A recent study supports the assumption that – at least on a relative scale – the effect factor, the potentially disappeared fraction and unfavourable conditions (mixture exposure) are related (Posthuma and De Zwart, submitted). For ecotoxicological effects of a mixture of toxic chemicals, several toxic mode of actions (TMoA) can be distinguished and the TMoA-specific disappearance of species, PDF_k, can be approximated by a sensitivity distribution *PAF* of acute L(E)C50-based species per toxic mode of action *k*, (Posthuma and De Zwart, 2006):

$$PDF_k \approx PAF_k^{L(E)C50} \qquad \text{Eq.5}$$

As the focus is on a marginal change in ecological damage due to marginal change in emission rate of a specific chemical *s*, the ecotoxicological effect factor for substance *s* in compartment *j* is obtained from $\partial PDF_{tox}/\partial C_s$, which is split into two factors:

$$E_{j,s} = \frac{\partial PDF_{tox}}{\partial C_s} = \frac{\partial PDF_{tox}}{\partial TU_k} \cdot \frac{\partial TU_k}{\partial C_s} = \underbrace{\frac{\partial PDF_{tox}}{\partial TU_k}}_{TMoA-specific} \cdot \underbrace{\frac{1}{HC50_s}}_{chemical-specific} \qquad \text{Eq.6}$$

TU_k is the effective toxicity of a pollutant with mode of action *k,* and C_s is the environmental concentration of substance *s* in compartment *j* with toxic mode of action *k*. $\partial PDF_{tox}/\partial C_s$ consists of a TMoA-specific part ($\partial PDF_{tox}/\partial TU_k$) and a chemical-specific part ($\partial TU_k/\partial C_s$). The toxic unit (*TU*) of chemical *s* with

concentration C_s (within TMoA k) is defined as C_s divided by HC50s, which is the Hazardous Concentration of substance *s* where 50 percent of the species is exposed above an acute toxic value (kg.m^3). The latter is the median of toxicity data (here acute EC50s) with respect to chemical *s*.
Entering the effective toxicity (TU_{k})), the TMoA-specific disappearance of species (PDF$_k$) and the hazardous concentration (here HC50) into equation 6 will result in effect factors for all receiving environmental compartments (*j*). If the specification per mode of action of the chemical under study is unknown due to the lack of data, the $\partial PDF_{tox}/\partial TU_k$ can be set at a typical value of 0.025 effect unit per toxic unit added on the basis of the number of chemicals within a TMoA (Van Zelm et al., 2007).

The characterization factor

Depending on whether the toxic mode of action is unknown or known, equations 7 and 8 can respectively be used for the calculation of characterization factors:

$$CF_{i,j,s} \approx F_{i,j,s} \cdot 0.025 \cdot \frac{1}{HC50_s} \qquad \text{Eq.7}$$

Or

$$CF_{i,j,s\in k} \approx F_{i,j,s\in k} \cdot \underbrace{\frac{\partial PDF_{tox}}{\partial TU_k}}_{TMoA-specific} \cdot \frac{1}{HC50_{s\in k}} \qquad \text{Eq.8}$$

In calculating the characterization factor, one should be aware of the need to check appropriateness of the (tabulated or calculated) units of the fate factor (year per m^3) and of HC50 (kg per m^3) as these might differ in practice. The dimension of *CF* is the disappeared fraction *PDF* times year per kg. $CF_{i,j}$ is specific for the compartment to which the substance is emitted (*i*) and to the receiving environmental compartment (*j*). As a number of fate factors (*F*) might be required, depending on the environmental compartments to which substance *s* is emitted (*i*) and transported (*j*), a number of characterization factors (*FC*) might be produced as well.

The impact score

The impact score ($IS_{i,j,s}$) for compartment *j* of chemical *s* emitted to compartment *i* is calculated by multiplying emission rate of chemical *s* to compartment *i* ($Q_{i,s}$) and the characterization factor $CF_{i,j,s}$:

$$IS_{i,j,s\in k} = Q_{i,s} \cdot CF_{i,j,s\in k} \qquad \text{Eq.9}$$

The equation results in the fraction of potentially disappeared species in compartment *j,* due to toxic effects of substance *s* as a result of a release of *Q* kg per year of substance *s* to compartment *i*. As *j* can refer to three compartments (terrestrial, freshwater and seawater), the impact categories are denoted as terrestrial ecotoxicity (TET), freshwater ecotoxicity (FET) and marine ecotoxicity (MET) respectively. Per receiving environment *j* a number of characterization factors, and thus impact scores, may exist if the substance *s* is emitted to different compartments *i*. All impact scores for the same receiving compartment *j* can be summed to come to a total impact score for respectively TET, FET and MET expressed in fraction of potentially disappeared species (per year). To calculate a total impact score, the impact scores per receiving environmental compartments (TET, FET, MET) first need to be multiplied by the number of species in the specific compartments before the scores can by summed to a total impact score. Dudgeon et al. (2006) estimated the total number of species per environmental compartment.

This method is based on the module for ecotoxicity from the ReCiPe life cycle impact assessment method (Goedkoop et al., 2009). It can thus be expanded relatively easily with other (background) environmental impact categories. ReCiPe is an LCA model that was developed by integrating various existing LCA models (CML LCA, Ecoindicator 99). The model was developed on the basis of consensus, initiated by a large number of LCA experts who expressed the desire to have a common framework for LCA. The ReCiPe model is now moving to become the standard LCA method used in various (international) LCA studies.

Table 4: Matrix overview of possible F, E, CF and IS because of different emitted (i) and receiving (j) environmental compartments and their interconnection

i/j	***j*, terrestrial**	***j*, fresh water**	***j*, sea water**
***i*, air (stratosphere, urban, rural)**	F_{air}, CF_{air}, Q/IS_{air}	F_{air}, CF_{air}, Q/IS_{air}	F_{air}, CF_{air}, Q/IS_{air}
***i*, water (waste, fresh, sea)**	F_{water}, CF_{water}, Q/IS_{water}	F_{water}, CF_{water}, Q/IS_{water}	F_{water}, CF_{water}, Q/IS_{water}
***i*, soil (natural, agricultural, industrial)**	F_{soil}, CF_{soil}, Q/IS_{soil}	F_{soil}, CF_{soil}, Q/IS_{soil}	F_{soil}, CF_{soil}, Q/IS_{soil}
Total	E_T; $IS_{air}+ IS_{water}+ IS_{soil}$	E_T; $IS_{air}+ IS_{water}+ IS_{soil}$	E_T; $IS_{air}+ IS_{water}+ IS_{soil}$

s = substance; *i* = compartment to which the substance is emitted; *j* = compartment to which the substance is transported and degraded (receiving compartment); k = toxic mode of action

3.5.3 *Step 4c: Environmental impact assessment based on a probabilistic exposure approach*

The most accurate method to determine the EIA is to combine the probability distribution of measured or predicted exposure concentrations and the species sensitivity distribution (SSD). The SSD enables one to perform an effect assessment from a relationship between the Potentially Affected Fraction of species (PAF) and the exposure concentration (Posthuma et al., 2002). Aldenberg et al. (2002) have demonstrated how such a distribution of exposure concentrations can be combined with SSD, which in itself is a probabilistic model for the variation of the sensitivity of an assemblage of biological species for a particular hazardous substance. While the method in the previous section is standardized (e.g., tabulated values relating to acute L(E)C50 data), the current approach can be tailored to the assessment problem, e.g., by selecting chronic data for both the BAU and the PS scenarios, depending on the context (i.e., what is the level of measured or predicted environmental concentrations in comparison to the set of available chronic- or acute ecotoxicity data).

The distribution of the exposure is determined by taking account of the uncertainty with respect to emission patterns and properties of the substance (especially the biodegradability). This information is used in multimedia environmental fate models of the category ‘Mackay-type’ (Mackay et al., 1985), like Simplebox, to produce a set of exposure concentrations in compartment j of chemical s. Application of software that is compatible to those box-models enables one to compute exposure concentration distributions (ECD_j) in compartment j of the modelled chemical.

Ecological impact is calculated from consideration of the (potentially) disappearance of species rather than their exposure above NOEC. As NOECs do indicate the actual impacts less clearly than, e.g., acute EC50s, for this purpose, other hazard indicators can better be used, for example, EC10, EC50 or LC50 data, and in this step there is a possibility to tailor the probabilistic approach to the data. For this reason, the SSD curve is drawn, based on acute effect concentrations (e.g., LC50s) instead of NOECs. Here, the choice of toxicity endpoints to derive the SSD can be tailored to the exposure distribution, i.e., the SSD should not be 'near horizontal' (lower and higher tail) given the exposure distributions of the two compounds. If exploration of this is considered, it can be borne in mind that the difference between $SSD^{L(E)C50}$ and SSD^{NOEC} for a compound is generically between half an order and one order of magnitude but - depending on the substance – other shifts amongst SSD-positions for different endpoint levels may occur (De Zwart, 2002). Figure 4 shows the combination of ECD with cumulative $SSD^{L(E)C50}$ (or PDF) curve to arrive at an estimate of the potentially disappeared fraction of species due to the exposure of an environmental compartment j to a concentration of chemical s. When – instead of SSD-L(E)C50 – the SSD would be derived for more sensitive toxicity endpoints, for example EC10, that SSD-curve would be positioned to the left of the one shown, implying a higher surface area (toxic impacted fraction of species not 1.6% but higher).

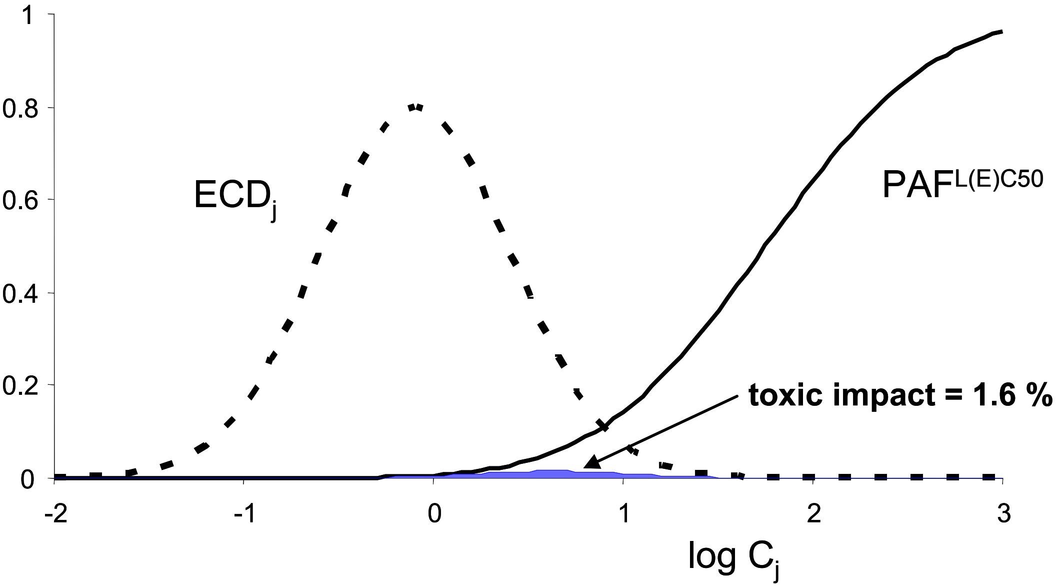

Figure 4: The potentially disappeared fraction of species due to exposure to chemical s in compartment j is equal to 1.6 %, when both the exposure (exposure concentration distribution (ECD)) and the sensitivity (SSD-L(E)C50) are distributed (respectively spatially and across species).

A probabilistic approach requires an evaluation of all emission characteristics, i.e., the spread of the emission rates to all relevant compartments and the uncertainty and/or variation in parameters in the fate and exposure modelling (box models). It is self-evident that the application of a probabilistic approach requires a minimum set of information to determine the minimum and maximum emission of the substances considered in the BAU and PS. If this information is not available and cannot be estimated, one could also apply the same method based on point source exposure estimatation (realistic or realistic worst case) instead of the probabilistic exposure distribution (the so-called 'semi' probabilistic approach). When all approaches chosen are the same as the ones described in the previous section, this approach is similar to the deterministic approach as described under step 4b. That is: the deterministic approach is a specific case of the probabilistic approach.

As mentioned in step 3, the focus of the EIA for PBT substances should at first be on secondary poisoning. To obtain a realistic distribution of the species sensitivity of predators (bird, mammal, fish), at least three or four chronic or reprotoxicity data should be available, to be integrated into one SSD. This can be a combined SSD from the different taxonomic groups bird and mammal (and possibly fish) - if combination in an SSD is acceptable - or an SSD derived for one (of the) taxonomic group(s) - separately. It is assumed that the data on chronic effects on vertebrate are often limited to mammals. In practice, this means that obtaining SSDs for secondary poisoning will often be impossible. If such is not the case, only a standard deterministic approach based on the calculation of RCRs out of the PEC and PNEC values, as estimated in steps 2b and 2c, can be taken. To make a conscious choice between BAU and PS, it would still be useful to apply this probabilistic approach for other relevant environmental compartments whenever feasible. However, these should always be reviewed alongside the RCRs of secondary poisoning and the PBT scores.

3.6 Step 5: Dealing with uncertainties

The assessment of environmental impacts of policy measures involves different types and sources of uncertainty. To understand the meanings of the end results, it is important to deal with these uncertainties throughout the environmental impact assessment process. Uncertainty is a multi-dimensional concept involving quantitative and qualitative dimensions (Van der Sluis et al., 2005). Uncertainty can be caused by, for example, the lack of data, errors in models, choices and assumptions, ignorance, and variability. Some of the uncertainties can be reduced by, for example, further data collection or generation of new data. Other sources of uncertainty, such as ignorance, differences of opinion or varying definitions are more difficult to reduce, but can nonetheless be identified and interpreted. For the environmental impact assessment of chemical substances we defined the three most important sources of uncertainties. These are the sources of uncertainty from which we expect the largest impact on the final results and conclusions of the assessment:

- the choices and assumptions made in the scenario definition (often only qualitative description possible);
- the release and exposure estimation, because of a general lack of information on this issue (dependent on data availability quantitative description may be possible);
- the translation of worst case risk estimates into realistic case impacts.

For the uncertainty assessment, we developed a standard table which can be used to identify and document the main sources of uncertainty for every case study. The table is based on Table 2 from Van der Sluis at al. (2005). The table allows the assessors to keep track of the choices and assumptions made, the data used, the uncertainties connected to these data and their expected influence on the end results in a uniform and consistent way. Since the end result of a case study is based on the comparison of environmental impacts of BAU and PS (i.e., the difference in environmental impact), the uncertainty table should likewise be based on the comparison between BAU and PS, and thus on relative uncertainties.

The basis of the table is presented below (Table 4). In principle the uncertainty analysis should start with the identification of the main sources of uncertainty. These can be identified on the basis of:

- previous research (what was the main bottleneck)
- sensitivity analysis (for quantitative data)
- group discussions among experts

The group discussions can tackle the issue from different perspectives: discussing along the steps in the assessment or along different types of uncertainty. The goal of the discussion is to reach consensus on the most important sources of uncertainty of the case under study. In the discussion, it is important to focus on the sources of uncertainty that are expected to play out differently in the BAU and PS.

Once most of the relevant sources of uncertainty are identified, the table can be filled out further. The table consists of quantifiable and unquantifiable dimensions. A tiered approach using different levels to deal with uncertainties (as described in the chapter on uncertainty analysis of the ECHA guidance, comparable with the horizontal axis of the tiered approach introduced in step 2) can be used when filling out the uncertainty table (ECHA, 2008c). The analysis on Level 1 is purely qualitative, the analysis on Level 2 is quantitative in a deterministic way and the analysis on Level 3 is quantitative in a probabilistic way. As far as possible, we suggest filling out the uncertainty table in a quantitative way, unless qualitative analysis is seen as sufficient (and proportional) in relation to the end results of the study. The first part (scope and scenario definition) will generally be filled out qualitatively because of its nature, in the main, the second part (input data and model parameters) should be filled out quantitatively. However, information on missing data or missing knowledge with regard to these data may still be described (only) qualitatively. The notes following Table 4 give instructions on how to fill out the table. Since we are looking at the difference in impact between BAU and PS, uncertainties that differ in influence on the scenarios may generally said to be more relevant than uncertainties with similar impacts on BAU and PS.

To increase the reliability (and reduce the subjectivity) of the uncertainty analysis, the parts based on expert judgement should be performed individually by a number of different experts. Generally, at least six experts are included in this type of expert elicitation, to obtain results that are assumed to be robust (Knol et al., 2010). However, this number is rather arbitrary chosen. In practice, the number could be reduced for valid reasons, for example, if there is general agreement among experts or if there are not enough resources (money, time) to involve a substantial number of experts. Together, the involved experts need to come to a general agreement on the qualitatively expressed uncertainties that will result in one uncertainty table.

Table 4: Overview of sources of uncertainty and error in the end results

Choice/assumption/input data used	**Quantitative or qualitative description BAU**[1]	**Quantitative or qualitative description PS**[1]	**Validity**[2]	**Consequence for the result**[3]	**Data source used and cause of uncertainty**[4]
Scope and scenario definition (choices and assumptions)					
(alternative) substance					
Included applications					
Replacement ratio alternative					
Scope of the impact assessment related to the restriction proposal (production, use, placing on the market)					
Included life cycle stages					
Production stage					
Formulation stage					
Use stage					
Waste stage					
Import/export					
Geographical scale					
Starting point in time of restriction					
Included time span of use					
Included time span of effect					
Assumed trend in use (import, export, production)					
Choice of relevant ecotoxic endpoints					
Choice of relevant					

environmental compartments					
…					
Input data and model/parameter uncertainties					
Included use amounts					
Release estimation					
Air					
Water (fresh/sea)					
Soil					
WWTP					
Secondary poisoning					
Exposure estimation					
Peak load vs. base load					
Combined exposure					
Used bioconcentration/ accumulation factors					
Used bioavailability factors					
Used conceptual model					
Used measurement data					
Used physical-chemical property data (Kow, Pvap, Sol, degradation rate constants)					
Environmental conditions (temp., rainfall, wind speed, water residence times, etc.)					
Hazard assessment					
Included species					
Included ecosystems					
Knowledge on sensitive species					

Specific vs general impacts					
Aggregation of impacts					
Choice on critical study(/ies)					
Used assessment/extrapolation factors					
…					

Note: the table format is based on Table 2 from Van der Sluis et al., 2005.

[1] *Quantitative or qualitative description of BAU and PS:* include the quantitative (i.e., value including units) or -if not quantifiable- a qualitative description of the parameter/variable (choice/assumption/input data) as used in the scenario (this column does not yet describe whether this parameter/choice/assumption is uncertain or not).

[2] *Validity:* in this column an indication should be given of the validity and tenability of the choice, assumption or input data used. The question here is how the parameter/variable as used in the scenarios relates to the real life impact situation. This will give an indication of the (un)certainty of the parameter and the possible incorrectness of the results comparing BAU and PS caused by this. Note: if the assessor thinks there is no uncertainty, this is also a possible outcome that should be noted in this column. One should try to express the validity in qualitatively terms at least. For example, if the choice is made to narrow down the geographical scope of the scenario because of limited data availability, this choice has a lower validity than if a more complete scope can be chosen. However, it might be tenable if the influence of the choice on the end result is assumed to be only marginal. If possible, the qualitative statements can be backed up by quantitative estimates of the uncertainty of that specific value.

[3] *Consequences for the end results:* the uncertainty or possible incorrectness of the choice/assumption/input data used in BAU and/or PS can have consequences for the end results. In this column one should try to:

a) Investigate the relevance of the source of uncertainty to the end result (are the end results sensitive to the source?). The source of uncertainty can be seen as more relevant if it is assumed to influence the conclusion of comparing the environmental impact of BAU and PS. If not assumed relevant, one does not need to fill out b).

b) Give an indication of the influence of the source of uncertainty on the end result: do we expect it to cause an under- or overestimation of the end result? In cases in which column 1 is filled out quantitatively, this column might also be filled out quantitatively, for example, by giving the spread, probability distribution (5th and 95th percentiles of distribution), e.g., of the number presented in column 1. If it is not possible to express quantitatively, one should try to indicate the influence on the end results in terms of ++; +; +/-; -; -- and ?; in which + presents an expected overestimation, – an underestimation, +/- not under- or over estimated and ? unknown consequences. In cases in which the consequences are filled out quantitatively, we suggest that the consequences are also represented in terms of + and –. to make the results ‘comparable’ (in relative terms).

[4] *Data source used and cause of uncertainty:* in this column, one should indicate what data source is used to come to the choice/assumption/input data used in the case study. The data density can be represented here as well. Possible data sources are: measurements, monitoring data, survey data, experimental data, model results, expert judgement etc.; might be further specified in, e.g., chronic or acute toxicity data, stating the model used. In this column, one can also present the cause of the uncertainty: lack of data or variability. When no specific data sources are used, one can give a short explanation here on which the expert judgement is based.

3.7 Step 6: Comparison of the scenarios

3.7.1 *Introduction*

As described in section 3.5, step 4 will result in estimates of the environmental impacts of BAU and PS. Outcomes may vary, depending on the method(s) used (4a, 4b, 4c):

1. PBT ranking (4a) results in a score for P, B and T, and their summed value, for both BAU and PS.
2. Deterministic approach (4b) results in an impact score, which is an estimation of the ecological impact for both BAU and PS in terms of the percentage of potentially disappeared fraction of species per environmental compartment.
3. Probabilistic approach (4c) results in an estimation of the ecological impact (impact score) for both BAU and PS in the fraction of disappeared species (or fraction of disappeared species per year) or another definition of impact (e.g., fraction exposed above their EC10) per environmental compartment.

Both 2 and 3 give impact estimates specified per environmental compartment. The three levels of approach result in relative and internally comparable impact scores for BAU and PS. In essence, the results of the different levels of impact assessment methods are not comparable, except when choices for method levels 2 and 3 would be exactly similar. Thus, comparisons of BAU and PS will first be made for all used impact assessment method levels separately. If more than one environmental impact assessment method is used, however, the different obtained impacts could and should also be analysed.

In the presentation of both the PBT and the deterministic/probabilistic impact assessment track, the major sources of uncertainties and their expected impact on the end result as presented in the uncertainty analysis, should be reflected to indicate the (un)certainty of the end results. Additionally, it might be informative to compare the impact estimates to the earlier calculated RCR values.

3.7.2 *PBT track*

For cases with persistent, bioaccumulative and toxic characteristics, PBT ranking is applied. The PBT scores of BAU and PS can be analysed as a total score (PBT-rank), or individual rankings for P, B or T can be compared. Note that the PBT scores *only* give relative information on the difference between P, B and T characteristics of substances. The scores do not have any absolute value and cannot be used to make a definitive decision on whether a substance fulfils the PBT or vPvB criteria or not.

When the total 'PBT score' of the alternative substance differs strongly from the score of the substance of concern, this method could be sufficient to make a judgement on the preferability of PS to BAU: one compound is clearly relatively (much) 'better' than the other regarding its potential to induce long-term impacts due to persistence and/or bioaccumulation potential, despite the fact that specific information on truly expected impacts is still lacking. Only major differences in emissions could affect the conclusion that one scenario is preferred to the other for environmental impact reasons.

When the total score differs only by less than, e.g., one unit, it becomes more difficult to make a clear distinction between BAU and PS, as the emission / exposure of the substances would become an increasingly important informative criterion. In this case, it becomes informative and relevant to review the separate scores of P, B and T next to the total PBT score. To include emission or exposure in the assessment, it is recommended (as mentioned in step 3) to perform an environmental impact assessment as well, to score the impact of the emission. This results in an impact indication for different relevant environmental compartments. Note that for PBT substances this EIA should at least include secondary poisoning. The individual P, B, T and impact of emission scores can be reviewed separately, as different 'weights' could be attached to the different parts on the basis of personal preferences. The weighing of a variety of different endpoints is already applied in various settings, e.g., in LCA (Guinée et al., 2001) and in the human health impact assessment expressed in DALYs (Murray and Lopez, 1997). Examples of weighing methods are swing weighing (Clemen, 1996) and multi criteria analysis. Both methods make use of the value judgement of a group of people (for instance, experts, policy makers, etc.). Note that – in practice - it is probably not possible to do a full impact assessment for secondary poisoning due to the lack of chronic exposure-effect data. In this case, the RCR values of secondary poisoning obtained in step 3 should be included in the preparation of the end results. As RCRs are not comparable by nature, one should be careful in using them. It may help to review the quality of the used PEC and PNEC data once again and include this information in the comparison.

Regarding the final interpretation of PBT-type scoring, different cases can occur in practice:

1. The PBT scores of PS and BAU differ significantly while neither scenario indicates a significant impact (or risk) estimate. In this case, it seems possible to draw a clear conclusion based on the PBT scoring, i.e., to identify the scenario with the lowest expected impact (lowest score).
2. The PBT scores of both BAU and PS are marginally different while the environmental impact (or risk) estimates of BAU and PS differ significantly. In this case, a clear conclusion can be drawn mainly on the basis of the impact estimates.
3. The PBT score for PS is significantly lower than for BAU, however, PS shows a significant environmental impact (or risk) and BAU does not (or the other way around). In this case, no clear conclusion can be drawn. The question is, then, what aspects we find most important or what aspect we think may give the highest impact. In such a case, one could, for example, weigh the P, B and T scores and the environmental impact estimates to decide which scenario is most favourable or look for other means (socio-economic impacts) to come to a conclusion.
4. There is no significant difference either for P, B and T scores or in impact estimates. This implies no environmental improvement resulting from the shift from BAU to PS.

Important remark for all above options: as we are dealing with one or more PBT substances for which it is difficult to determine impacts due to the nature of the substances, one should be *very careful in drawing conclusions* as relevant endpoints, and thus impacts, might be missing in the assessment. Care should especially be taken if P and B sores are high and secondary poisoning could not fully be included in the assessment.

3.7.3 Deterministic and/or probabilistic impact assessment track

The probabilistic and deterministic impact estimates should generally indicate the same trend in results when comparing the impacts of BAU and PS. If this is not the case, there might be an error in one of the estimations, so they should be checked. In general, the impact estimation of the probabilistic method will be more accurate and meaningful than the deterministic approach, especially since the third method allows for ‘tailoring the effects assessment to the specific cases’. If marginal differences occur between impacts of BAU and PS, it should be questioned whether the difference is significant. When the analysis is done in a probabilistic manner, the results will show whether the difference is significant. When the deterministic approach is used, it may be less clear whether the impact estimates differ significantly. In that case, one should estimate the significance of the difference based on expert judgement taking into account the uncertainties as analysed in step 5.

4 Case studies

4.1 Introduction and choices

To test and further work out the methodology, three case studies have been carried out parallel with the development of the methodology (Table 5):

- nonylphenol and nonylphenol ethoxylates
- zinc and PVC in gutter systems
- HBCDD and TBECH/TCEP in EPS

The case studies were chosen to enable a check on the practicability and workability of the methodology under development, and to guarantee a potential ‘broadness’ in the use of the methodology. The case study chemicals chosen for this project are presented in Table 5 below. The cases include three very diverse substances representing a range in possible hazard, exposure, and possible impact as well as practical issues, such as data characteristics and availability. The methodology developed was thus challenged to deal with differences in hazardous effects, environmental impacts, uncertainty and data availability. moreover, possibilities to achieve results in case of low data availability or differences in data availability between BAU and PS can be investigated.

All three case studies applied the full methodology. However, for some case studies, a specific focus was chosen to test and work out a particular part of the methodology more specifically.

In the case of nonylphenol and nonylphenol ethoxylates, two different environmental impact assessment methods were tested: the deterministic (step 4b) and the probabilistic method (step 4c). Moreover – due to it being an historic case – some monitoring data on environmental concentrations could be included in the case to check the correctness of the estimates on exposure with the real-life situation after introduction of the restriction.

For the zinc case, special attention was given to the uncertainty analysis, as the data availability for BAU and PS differed. For this case also, some attention is given to possible expansion of the assessment with other environmental impact categories, as the substance of concern (zinc) differs a lot from the reviewed alternative (PVC + additives).

In the case of HBCDD – being a persistent and bioaccumulating substance – the PBT ranking method was tested alongside the probabilistic impact assessment method. In this case, again, special attention was given to the uncertainty analysis, as data availability for both BAU and PS is very limited.

Table 5: Overview of the case studies and their characteristics

Criteria	**NP/NPE and AE as detergent**	**Zinc and PVC gutter systems**	**HBCDD and TBECH/TCEP in EPS**
Hazardous effect/mode of action BAU and PS	Similar	Different	Similar/different depending on alternative
Relevant compartments	Water	Soil and water	Secondary poisoning
Data availability (and uncertainty)	Sufficient for BAU and PS	Sufficient for BAU, limited for PS	Limited both for BAU and PS
Validation with measurement data	Possible for environmental concentration as historical case	Might be possible	Not likely
REACH regime	Yes	Yes	Yes

4.2 Summary of EIA findings in the case studies

This section outlines the output of the case studies regarding the assessment of impacts via the proposed approaches and methods. The full descriptions of the case studies can be found in Appendices B, C and D of the report.

4.2.1 The case on Nonylphenol

Nonylphenol (NP) and NP ethoxylates (NPE) are considered priority substances (793/93/EEC) given large quantities produced and used annually, high toxicity to aquatic organisms, and low biodegradation concerns. Furthermore, NP is classified as an endocrine disruptive compound, displaying some estrogenic activity. Restrictions are already in place for NP and NPE, making this a case where an historical restriction decision is considered in the context of SEA under REACH. Alcohol ethoxylates (AE) are considered as alternative compounds. The two scenarios studied were ´no restriction of the use of NP and NPE in detergents´ versus complete replacement of the detergent use of NP and NPE by the use of a variety of AE homologues, and not by other kinds of detergents. Emission levels of AE were varied, yielding net results for different AE use scenarios (variation in replacement ratio NP/E:AE).

Expected and reviewed measured concentration data in water, sediment and soil were collected from models and data review.

Hazard data were collected from databases and literature. They were re-calculated if necessary by means of equilibrium partitioning of hazard data for relevant environmental compartments.

According to the case study characteristics and for methodology testing purposes, deterministic and probabilistic assessments were made for both scenarios.

The assessments first showed that RCR values for NP and NPE were highest for sediment dwelling organisms in the BAU-scenario. All RCRs remained below the value of 1 for the alternative scenario, with 70% reduction of NP due to the restriction measure. Data for endocrine disruption effects were scarce, but they did not change the implication of this RCR pattern (i.e., RCR remains probably less than 1 under the Policy Scenario). The BAU scenario resulted in higher RCRs than the PS. The compartments surface water, sediment and soil were selected to be included in the impact assessment, as RCRs were larger than 0.8. Secondary poisoning was not further included, as no risks were indicated there.

In the impact assessment, the difference between the deterministic impact scores for the Business As Usual scenario were 0.14% larger than for the Policy Scenario. This suggested a slight difference in impact scores, with the PS implying slightly less affected species in freshwater systems. In the probabilistic assessment, the calculated toxic pressure levels (PAF) were generally (water, sediment, soil) lower for the PS scenario than for the BAU scenario.

From both assessments, the AE scenario yielded lower values for both SI and PAF, be it marginally. This is not surprising, given the relatively low RCRs. The (relatively) low exceedance of the original RCRs, which triggered the impact assessment, suggests that impacts are not easily visible in field studies with such exposure levels (see, e.g., Mebane et al. 2011), nor are they expected to be in terms of predicted species loss (as used in the impact assessments). Nonetheless, since the relative values of both SI and PAF (deterministic and probabilistic methodologies) are lower, there is cause to consider whether the alternative PS is of lower impact than the BAU scenario.

In the uncertainty analyses, firstly, the conclusion could be drawn that the selection of alternative AE compounds (replacing NP and NPE) did not matter for the general conclusion. Furthermore, qualitative or quantitative aspects of uncertainty were assessed, according to the proposed table, which was filled out. The uncertainty assessment did not change the conclusion of the environmental impact assessment. There is a consistent albeit slight difference between expected impacts (at the level of species probably disappearing) of continued use of NP and NPE, which is larger than seen after replacement by AE (various possible compounds).

Due to the focus of the case study on method development and testing for SEA, these results need not be considered as final. Further attention to specific mechanisms of action, like endocrine disruption, could show larger divergence amongst scenarios, and focus on more sensitive endpoints (not species probably disappearing but species affected beyond, e.g., their chronic EC50 or NOEC) could substantiate the relative difference between the scenarios better.

4.2.2 *The case on Zinc*

In the Netherlands, zinc is widely used in rain gutter systems. It has been shown that the leaching of zinc to surface waters results in an exceedance of the maximum allowable concentration, e.g., in some regional surface waters. Zinc gutters can be replaced by PVC gutters. Two scenarios are included in the case study: the scenario in which zinc gutters are used in a typical residential area (BAU), and the scenario in which zinc gutters are restricted and replaced by two types of PVC gutters in a period of twenty years (rigid and flexible type, containing zinc and DEHP as additives). Replacement ratio is based on the estimated required surface, thickness and assumed percentage of additives.

Major release and exposure from gutter systems is caused in the use stage, and therefore, the case study focuses on this stage. Release estimates were made on the basis of available data (zinc) and assumptions (PVC). Subsequently, the exposure was calculated. Exposure of zinc and DEHP is assumed to mainly affect the aquatic environment. Besides that, some of the DEHP is assumed to end up in sediment.

Hazard data were collected from literature and were re-calculated, if necessary, by equilibrium partitioning of hazard data for relevant environmental compartments.

Both for zinc and DEHP, environmental hazard characteristics are based on ecotoxicity only. Therefore, both the deterministic and the probabilistic impact assessment methods are feasible. For this case study, the 'semi'-probabilistic approach (probabilistic effect assessment) based on SSDs was applied. Note that if the tiered approach were applied consistently, the deterministic approach would presumably be sufficient.

Reviewing the water compartment, the first assessment shows that RCR values for zinc shift from 2.0 in BAU to 0.006 in PS after full replacement of zinc gutters with PVC gutters. With regard to sediment and DEHP, it can be noted that due to an increase of the exposure of DEHP, the RCR for DEHP shifts from 0 to <0.001. In other words, the restriction of zinc gutters will significantly reduce risks in terms of RCRs. As the RCR of BAU for the water compartment is larger than 0.8, the impact assessment for this environmental compartment will be continued.

The impact assessment gives a potentially affected fraction of species of around 15% for BAU and of <1% for PS. This suggests a significant environmental improvement for the aquatic environment if zinc in gutter systems is replaced by PVC gutters. This level of improvement was not shown by the relatively low RCR values shown in the earlier risk assessment.

The uncertainty analyses indicated sources of uncertainty that might have an influence on the end results. Firstly, the additives used in PVC gutters are uncertain regarding their influence on the outcomes. Although zinc and DEHP are plausible additives, other additives might also be used. As geographical scale, a residential area was taken with a relatively high gutter density, resulting in an overall overestimation of exposure and thus impacts. In the choice of relevant environmental endpoints, only general acute ecotoxicity was included. Further attention to specific mechanisms of action (e.g., endocrine disruption) and chronic studies especially for DEHP might influence the end results. The release estimation for PS is fully based on assumptions resulting in a possible over- or underestimation of the environmental concentration of PS. The overall effect of these major sources of uncertainty can affect the results in two directions.

The study shows a significant environmental improvement for the water compartment resulting from the shift from zinc to PVC gutters. Human health effects, e.g., from DEHP (being the major concern of the substance) are not included in this case study. However, one should bear in mind that it is a case study performed for methodology testing purposes.

4.2.3 The case on HBCDD

Hexabromocyclododecane (HBCDD) is used as flame retardant in, e.g., expanded polystyrene (EPS). HBCDD is found to be hazardous to human health and the environment. Looking at environmental concerns, the substance is toxic and non-readily degradable and, therefore, complies with the REACH criteria for a PBT substance. In this case study, a variety of scenarios is reviewed. The Business As Usual (BAU) scenario assumes the continuous use of HBCDD in EPS. Besides that, different Policy Scenarios (PS) are reviewed representing the restriction of HBCDD. Two Policy Scenarios assume the replacement of HBCDD with other flame retardants: dibromoethyldibromo-cyclohexane (TBECH, PS1) and tris(2-chloroethyl)phosphate (TCEP, PS2). For PS1 and PS2 replacement ratios of 1:1 are used, assuming comparable fire resistance of the flame retardant materials.

Release estimates were made on the basis of available data (RAR, HBCDD) and assumptions (TBECH). Subsequently the exposure was calculated using the spread sheet version of EUSES. The assessment focuses on the water compartment and on secondary poisoning, as PBT substances are likely to accumulate in the food chain.

Due to the lack of sufficient experimental data, the hazard data for both HBCDD and TBECH were mainly derived from QSAR and ECOSAR models.

According to the case study characteristics, the PBT ranking method and the semi-probabilistic impact assessment method were applied. The PS3 scenario was only included to test the PBT ranking method. Therefore, the semi-probabilistic impact assessment method was not applied to this scenario.

Reviewing the water compartment, the assessment showed low RCR values, with only marginal differences between BAU and PS. For secondary poisoning the assessment shows an RCR far over 0.8 for BAU (22.0) and of almost 0 for PS2. Unfortunately, we were not able to calculate RCR values for PS2. According to these results, the probabilistic impact assessment should be continued for secondary poisoning. For methodology testing reasons, the water compartment was reviewed as well.

The PBT ranking shows very high scores of HBCDD (BAU) for B, P and T, TBECH (PS1) gives intermediate scores and TCEP (PS2) gives relatively low scores. This suggests a reduction of concern when moving from BAU to PS1 or PS2. The (semi-)probabilistic impact assessment for the aquatic compartment shows – as expected on the basis of the RCRs – very small impacts for BAU (0.16) and PS (0.125 and 0.035). Unfortunately, it was not possible to perform the probabilistic impact assessment for secondary poisoning, due to the lack of hazard data for secondary poisoning. The RCR calculations are thus the best we can get reviewing secondary poisoning. Reviews of both the PBT ranking and the RCR values for secondary poisoning, imply a substantial environmental improvement from the shift from HBCDD to TBECH or TCEP. What this means in terms of actual environmental improvement (e.g., lost species) could not be quantified.

The uncertainty analysis revealed a number of both more and less important sources of uncertainty. The main cause of uncertainty in this case study is assumed to be the lack of information on the possible alternatives of HBCDD. Discussions on the technical feasibility of alternative flame retardants for EPS are on-going, and the feasibility of the substances included as alternatives in this case study is also being debated. Lack of release, exposure and hazard data for these alternative substances bring in more uncertainties, as many assumptions had to be made to fill in this data gap. The uncertainties could, therefore, either give an under- or over estimation of the end results.

4.3 Methodological lessons from the case studies

This section gives an overview of the application of the methodology to the three case studies, thereby deriving methodological lessons from the technical execution of the case studies. Table 6 summarizes what was actually done in the case studies, what problems and discussion points emerged in preparing the case studies and applying the methodology, and finally what was learned from the case studies regarding the EIA-methodology. The full description of the case studies can be found in Appendices B, C and D of the report.

Table 6: Methodology applied in the case studies: NP and NPE as surfactant, zinc in gutter systems and flame retardant HBCDD in EPS

Case study	***NP/NPE***	***Zinc***	***HBCDD***
Step 1: Scope and scenario definition			
What is done	Historic restriction case of NP/NPE vs. AE detergent. C10EO3 as representative of the AE group. 1997 (NP/NPE) and 1999 (AE) base years, no trend taken into account. Europe. Various replacement ratio included (NPE:AE, on weight basis) 1:1; 1:0.5 and 1:2. All life cycle stages included. Water, sediment, soil included, sec. poisoning only partially included.	Zinc vs. PVC gutter systems. DEHP and zinc stabilizer as additives to PVC gutters. Base year 2011, total replacement in twenty years. Replacement rate based on required surface. The Netherlands chosen as geographical scale. Only use stage included. Water and sediment included as relevant environmental compartments.	HBCDD vs. TBECH or TCEP flame retardant in EPS. Used amounts based on 2006 (BAU) and 2007 (PS). Not accounted for planned policy measures and other trends in BAU and PS. Not accounted for any transmission period. Replacement ratio 1:1. All life cycle stages included except the waste stage. Europe is taken as geographical scale. Water and sec. poisoning included as relevant environmental compartments.
Problems, discussion points	- What to do when BAU or PS include a group of substances and with that include a wide range in exposure and hazard characteristics. - Lack of data results in many assumptions (alternative, replacement ratio, etc.), what is acceptable? - What to do in case no clear alternatives are available; would this be a reason to stop the assessment?		
What is learned	- The importance of including realistic alternatives in PS for real life value of the results. - Importance of determining the relevant life cycle stages, the relevant environmental compartments and hazard indication upfront in the process to correctly target the assessment. - Data deficits can often (always?) be solved by making assumptions. This possibility should be handled with care as it will raise uncertainties to possibly unacceptable levels. - Plausible alternatives that are very different in character (like glass wool in case of HBCDD) ask for a broader approach in the assessment, for example, including the isolation material and other environmental impact categories in the case of HBCDD. This would be possible when the methodology is further expanded. - One should be very aware of the assumptions made in scenario definition as		

Case study	***NP/NPE***	***Zinc***	***HBCDD***
	they might include a serious level of uncertainty.		
Step 2: Exposure and hazard determination			
What is done	Analysis at tier 3 or 4. Exposure based on (worst case) modelling checked by some measurements. Hazard estimation based on large (BAU) and minimum (PS) number of toxicity data (>5 vs. 3).	Analysis at tier 2 or 3. Release and exposure estimates calculated on the basis of leaching rates BAU, assumptions made for PS. Hazard estimation based on large data and medium number of toxicity data (>5 vs. 4).	Analysis at tier 1 or 2. Release and exposure estimates based on earlier studies (ECHA, 2009 and OECD, 2009) and EUSES. Hazard estimation based on minimum toxicity data complemented with QSARs calculations.
Problems, discussion points	- Probabilistic exposure estimate difficult due to the fact that we are dealing with a group of substances. Lower tier approach was chosen because of the assumed proportionality to the produced results (NP). - Discrepancy between theoretically possible and calculated concentration of DEHP in water. Solved by including sediment compartment (Zinc). - Problem of very low hazard data availability (HBCDD).		
What is learned	- Tier chosen can change during the process as at this stage in the process one cannot always determine what is appropriate/necessary to come to conclusive results.		
Step 3: Determination of endpoints and assessment method			
What is done	PBT not assumed relevant. Deterministic approach could be sufficient. Probabilistic approach added for testing purposes. RCRs BAU >0.8, RCRs PA <0.8: assessment continued to quantify the difference.	PBT not possible (zinc). Probabilistic approach. Choice for approach not made consciously. RCRs BAU >0.8, RCRs PA <0.8: assessment continued to quantify the difference.	PBT relevant. Probabilistic approach targeted to (at least) secondary poisoning. RCR BAU sec. poisoning >>0.8; RCR PS sec. poisoning could not be derived for most scenarios: assessment continued.
Problems, discussion points	- Difficulty in choosing the right tier of assessment at this moment in time. Way forward could be to always take the deterministic approach and expand to higher tier if that proves to be necessary. - Relevance of continuation of assessment when RCRs already show a difference BAU and PS. - What cut-off RCR to apply?		
What is learned	- Limited data availability for PS can hamper the decision whether and how to continue the assessment. - Importance of including secondary poisoning in case of PBT substance. - More transparent deterministic approach seems better known and accepted in the field of toxicology than the less transparent deterministic approach. This does not necessarily mean that the probabilistic approach is always the most appropriate method. - Incentive to continue to impact assessment is not only based on data availability and comparison BAU and PS, but also by the need to quantify the difference and the context in which the results are to be used.		
Step 4a: Impact assessment – PBT ranking			
What is done	-	-	Applied on the basis of QSARS for HBCDD, TBECH and TCEP.
Problems,	- A very limited number of substances included to test the PBT ranking method		

Case study	***NP/NPE***	***Zinc***	***HBCDD***
discussion points	and get a good feeling on the actual value of the results obtained by this method. - The PBT ranking method gives relative results that are only comparable in case compatible input parameters are used. Results using PNECs will differ from results using QSARs. One should therefore be very careful in choosing input parameters.		
What is learned	- It would be very helpful to further test the methodology on a range of substances to get a better feeling of the meaning of the scoring results. - Further testing of the T scoring formula is especially required, as this was not tested earlier in other reports; important point in the testing is the range in PNECs for which the formula is sensitive (shows changes between 0-1).		
Step 4b. Deterministic impact assessment			
What is done	Applied for the water compartment.	-	-
Problems, discussion points	- The fact that the method is a black box can give problems, as it is hard to recognize possible mistakes, get a grip on the meaning of the results and indicate the uncertainties around it. - Extensive simultaneous testing of methods 4b and 4c can help estimate the actual value of this deterministic method.		
What is learned	- The input parameters are not always easy to find as tables provided by Huijbrechts (2004) are not exhaustive. If not available, parameters can be calculated using the ReCiPe methodology (Goedkoop et al., 2009), however, this requires expertise. - As only very few parameters are used in the calculation, one should be very certain about the actual values. - As units of input parameters differ in practice, one should be very conscious of the units of the used parameters when using the method.		
Step 4c. Probabilistic impact assessment			
What is done	Applied for water, soil and sediment. semi-probabilistic: using point source exposure estimate.	Applied for water. semi-probabilistic: using point source exposure estimate.	Applied for water. Applying for secondary poisoning was not possible because of lack of hazard data. semi-probabilistic: using point source exposure estimate.
Problems, discussion points	- What is the minimum data set required to produce an SSD? - Relevance of higher tier approach based on probabilistic exposure estimate (NP). - Lack of hazard data made it impossible to perform impact estimation for secondary poisoning, which is required for PBT substances. Because of this, the assessment gives an incomplete picture (HBCDD).		
What is learned	- SSDs based on NOECs do not give information on actual impacts, to get impact estimates LC/EC/HC (50) data need to be used (Zinc). - In practice. EIA for secondary poisoning (for PBT substances) may not be possible because of limited chronic toxicity data to derive an SSD. - In general, three or four hazard data are required to derive an SSD. However, one will always get more information using more than one hazard input, which would plead for preparing an SSD with a higher level of uncertainty out of fewer hazard data instead of only an RCR estimate.		
Step 5: Uncertainty analysis			
What is done	Analysis at low/intermediate	Analysis at low tier/level 1. No	Analysis at low tier/level 1. No quantitative

Case study	***NP/NPE***	***Zinc***	***HBCDD***
	tier/level 1 or 2. Quantitative sensitivity analysis on replacement ratio. No sensitivity analysis on choice representative AE alternative as this is assumed to fall well within the range of the replacement ratio. Uncertainty table mainly filled qualitatively based on expert judgement (only two experts involved).	quantitative sensitivity analysis to indicate importance of sources of uncertainty. Uncertainty table filled qualitatively based on expert judgement (only two experts involved).	sensitivity analysis to indicate importance of sources of uncertainty. Uncertainty table filled qualitatively on the basis of expert judgement (only two experts involved). The relevance of the sources of uncertainty were scored using a ranking of 1-5.
Problems, discussion points	- How to decide what level of detail is required in the uncertainty analysis and what is to be done quantitatively and what qualitatively. In the case studies this was based on the available data and the available time. However, this leaves a lot (too much?) open to the interpretation and resources of the assessor. In the case studies, this resulted in minimum uncertainty analysis. - For all uncertainty tables the two experts involved came to different results. In most cases however, the experts indicated similar major sources of uncertainty for the case studies. - Gathering enough experts to join the expert elicitation might be a problem in practice. The relevant question here is whether experts require a certain background to be able to fill out the table or whether the table can be filled out on the basis of the information provided by the text description of the case study.		
What is learned	- In all cases, the uncertainty of PS is higher than of BAU (although there are gradations in the uncertainty and the consequences to the end results: NP= uncertain but acceptable versus HBCDD= uncertain probably not acceptable). Applying similar assessment methods and similar tiers is necessary to come to comparable results, the appropriateness of which can be discussed. Also, proportionality should be included in the decision making. - What is possible in terms of uncertainty analysis is not always proportionate (NP). - Importance of using quantitative sensitivity analysis wherever possible to indicate the relevance of sources of uncertainties and possible effects to the end results. For example, for the HBCDD case experts did not always agree on points that could be checked quantitatively. Only if sensitivity analysis is not possible, expert elicitation should be used.		
Step 6: Comparison of the scenarios			
What is done	Comparison made internally (BAU and PS) and externally (deterministic and probabilistic approach). Results in absolute and relative improvement. Major uncertainties reflected.	Results presented in absolute improvement. Also other environmental impact categories added to the results. Uncertainty analysis reflected in the result.	Comparison of PBT ranking on individual and total scores. Impact estimates for secondary poisoning not possible and therefore felled back on RCRs. Major uncertainties reflected.

Case study	***NP/NPE***	***Zinc***	***HBCDD***
Problems, discussion points	- How to reflect the uncertainties in the final results not so easy. - What is the actual (and practical) meaning of the end results of the different methods, when are impacts and impacts differences significant. - How to combine the 'apples and oranges' of the different methods to total impact scores. The results of, e.g., the PBT scores and the RCRs in HBCDD case give similar results (PS is better than BAU), but what to do if results of the two methods yield contradicting results? - Impacts presented in the NP case differ enormously from the estimation made by WCA environment (WCA, 2011) for this substance. The reason for this difference could not be traced and required further contact with WCA environment.		
What is learned	- There is not necessarily a relation between indicated risks (RCRs) and impacts. Indicating that there is a risk does not necessarily mean that there is an impact. For a better understanding of this relation, RCRs should be reflected in the comparison of the scenarios alongside the impact estimates. - Incompleteness of the impact assessment needs to be indicated in the results when relevant. - When calculated impacts are very low, relative presentation of the impact difference can be misleading. Absolute numbers should therefore always be presented. - Including other environmental impact categories can be very relevant and gains importance as differences in characteristics between BAU and PS increase.		

5 Concluding thoughts, discussion and follow-up

5.1 Concluding thoughts and lessons learned

Concluding thoughts

In an SEA, the expected socio-economic impacts of a policy measure (PS) are compared to the expected impacts of the current situation in which no policy action is introduced (BAU). The socio-economic costs of, for example, a restriction proposal are compared to the benefits of the restriction in terms of the reduction in impact on human health and the environment. The generally applied chemical safety assessment under REACH gives realistic worst case estimates of risks, that are incomparable by nature and do not inform about possible expected impacts of the production, use and waste stage of a chemical substance. Risk Characterization Ratios (RCRs) give us information on the magnitude of the risk, but not on the absolute adverse effects on populations in ecosystems, so-called environmental impacts. This report is an attempt to bridge this gap between risk estimates and impacts. The report introduces a comparative methodology providing a relatively simple framework and practical guidance to estimate the environmental benefits of policy measures. The methodology is new in its tiered approach that allows for the selection of the possible and appropriate manner and level of detail of the assessment and in its systematic way of dealing with uncertainties. This report thereby tries to contribute to the socio-economic analysis in the context of REACH restrictions or authorisations. However, due to the narrow scope of the study, focusing on the quantification of environmental impacts, the report only contributes to part of the full socio-economic analysis. E.g., human impact assessment is outside the scope of this report, but reference is made to the RIVM report published in 2008, in which an extensive analysis of the quantification in the human health impact assessment of policy measures for chemicals in non-food consumer products was performed (Schuur et al., 2008).

To further investigate the value of this environmental impact assessment methodology for SEA, expansion of the scope towards other socio-economic impact categories (human health, costs to industry, society, etc.) and valuation methods will be needed. In this broader comparison of impacts, the actual value of the work done can be further tested.

Lessons learned

This report gives a methodological framework for environmental impact assessment of chemicals in the context of REACH. Developing and testing of the methodological framework increased our understanding of the possibilities and impossibilities of environmental impact assessment and showed the major problems, for example, on data availability, uncertainty and the actual meaning (or practical value) of the end results. The exercise, however, also showed that it is possible, even with a limited amount of data, to move from risk indicators to impact indicators that are more useful in the context of the socio-economic analysis. It showed the importance of a robust uncertainty analysis in an assessment where a variety of input data, models and methods are used and connected, to understand the actual meanings of the end results. The methodological framework is another step meant to help the quantification of impacts to be used in the socio-economic analysis of REACH instruments in addition to the work that has already been done on this subject (as has been described in chapter 2). A follow-up of this work – both methodological and in terms of practical experience - will be helpful to further develop and improve the socio-economic analysis underpinning REACH restriction and authorisation dossiers.

5.2 Discussion

In the development of this methodology framework and in testing the framework using case studies, a number of discussion points came up regarding the methodology framework, the methods used, the uncertainties in the methods and the usefulness of the framework and methods for policy support. These will be discussed below.

Methodological aspects

The framework allows a tiered, consistent approach towards environmental impact assessment to be used as input for a socio-economic analysis of the Policy Scenario (PS) as compared to the Business As Usual scenario (BAU). Depending on the data availability, first indications of risks and impacts and the final purpose of the assessment, the framework helps decide whether it is necessary, possible and valuable to perform an environmental impact assessment and what level of detail is appropriate. The case study on nonylphenol, for example, shows that it will not always be necessary (or proportional) to perform a full probabilistic environmental impact assessment. For this case study, too, the simplified deterministic approach or an approach based on point estimates of exposure showed to be sufficient for decision making. This tiered approach enables a cost- and time-efficient way for environmental impact assessment of chemicals as decision support instrument under REACH.

In step 3 of the methodology, a cut-off RCR value of 0.8 was introduced to decide whether it is useful to do an impact assessment. The motive for this choice is that below the RCR of 1 no risk is considered to be present and thus no impact either. To account for some uncertainties in the estimation of PECs and PNECs, however, the cut-off was set on 0.8. As stated in the methodology description, this is an arbitrary choice that needs to be discussed and adjusted on the basis of further experiences. Looking at the RCRs and impact estimates of the case studies, RCRs of below 0.8 indeed do not show significant impacts. However, RCRs over 0.8 do not always show significant impacts either (case studies and Mebane et al., 2011). More test cases in which the relation between RCR values and estimated impacts can be evaluated would be required to indicate a better funded cut-off RCR value. Note that the accuracy of the cut-off RCR value will depend on the uncertainties of the PEC and PNEC estimates (worst case versus realistic case), as well as on the possibility that specific endpoints (like endocrine disrupting effects) might occur. Available ecotoxicity data should be scrutinized in relation to the essential features of a compound and its alternatives, to avoid that RCRs trigger ‘no attention in SEA’, while specific effects might occur.

The proposed methodology includes three different environmental impact assessment methods in step 4. The PBT ranking method is exclusively developed for substances that are indicated as persistent, bioaccumulative and toxic. Moreover, there are two methods for environmental impact assessment that can be used to estimate the impact of toxic characteristics of the use of substances. These methods are basically more or less comparable and can also be used to complement the PBT ranking with the focus on secondary poisoning.

The PBT ranking method is based on the work of Rorije et al. (2011) for the identification of potential POP and PBT substances. Three different equations are used to indicate whether the substance under study is likely to fulfill the PBT criteria, thereby giving an estimation of the seriousness of the relative persistence, bioaccumulation and toxicity of the substances under consideration. The equations to indicate the level of persistence and bioaccumulation of substances are derived from the report of Rorije at al. (2011) and are tested and discussed in this report. For this methodology, an additional equation to score toxicity was introduced to give a more complete picture of the hazardous characteristics of a substance that can potentially affect the environment. The equation to score toxicity centralizes around a PNEC of 1 µg/l and reacts sensitively in the range of values between 0.1 and 10 µg/l. At this point in time, the method is only tested using a very low number of substances in the HBCDD case study. Much more extensive testing of the T score is desirable to assess whether the scaling and the range of the equation is appropriate for its goal in this methodological framework, and to get a better feel for the meaning of the scoring results.

Data availability

As mentioned earlier, data availability is a major decision criterion in the methodological framework. An important question in the development of the framework is the nature of the minimum data set required. The results of this report indicate that a uniform answer about the data requirement for environmental impact assessment is difficult to give, as the minimum data requirement is seen to be case-specific. It depends, for example, on the context in which the results will be used (as this will determine what is 'sufficient' and what is not) and also on the difference in expected impacts between BAU and PS (as this will determine the required accuracy). To purely compare environmental impacts of BAU and PS scenarios, relative impact estimates are sufficient, and for such cases fewer data will be required, provided data availability and uncertainties are comparable for both. However, to be of use in the broader context of the socio-economic analysis, a more detailed analysis will be preferred that gives a better indication of the absolute level of environmental improvement, which could be potentially comparable with other socio-economic impacts. The required accuracy of the results is connected to the differences in the (expected) impacts of BAU and PS, but also to the overall size of the impacts of BAU and PS and the context in which the results are used (the latter being connected to the issue of sufficiency). When the difference in impacts between BAU and PS is smaller, a higher accuracy of the results is required than in cases where the difference is substantial. However, when impacts of both BAU and PS are very small, as is the case in the nonylphenol case study, higher accuracy will not change the conclusion that the policy measure under study will only marginally reduce the impact to the environment.

The experiences gained with the case studies show a wide variety in available input data, and in all cases, end results in terms of relative environmental improvement are obtained. All case studies seem to provide enough data to conclude on the difference between BAU and PS and provide an estimation of the level of improvement. For the context of SEA, however, estimates of the NP case are assumed to be more useful/reliable in absolute terms than, for example, the HBCDD case, just as the data availability (and reliability) for the nonylphenol case is much more extensive than for the HBCDD case. For HBCDD, for example, the assumptions made on alternatives because of the lack of data on this aspect and the inability to perform the environmental impact assessment for secondary poisoning minimizes the practical value of the end result of this case study.

Often, the data availability for the PS is less than that for the BAU scenario. This difference in data availability might give problems in the comparability of the impact estimates of BAU and PS. By using similar input data and methods for BAU and PS in the different steps of the methodology and by including quantitative uncertainty estimates (distributions), the comparability in results is increased. Although comparability cannot be fully guaranteed, the case studies show that it may be possible to come to comparable impact estimations in spite of a serious lack of data. Only in the case of HBCDD, it was not possible to estimate PNECs, and thus RCRs and impacts for all Policy Scenarios.

Uncertainties

A major problem in the (environmental) impact assessment of chemicals is the uncertainties in, for example, exposure or actual effects caused by the production and use of specific chemicals. Also, in cases where some information is available on the hazardous characteristics of the substance, its use, emission and exposure, it will be hard to get an accurate estimate of the impact that reveals the full causal chain, from the life cycle of the chemical towards environmental impacts. Consequently, chemical policies usually rely on risk assessments that take a realistic worst case approach, thereby claiming to protect the environment against hazardous impacts. However, when insight in socio-economic impacts is required (or desired) to underpin a policy measure, for instance, for a restriction or an authorisation proposal, one needs to take a step from the realistic worst case risks to more realistic case impact estimates. In taking this step, both more and other types of input data are required, and thus more pressure is put on the uncertainty analysis of the assessment (one cannot ‘simply’ confine oneself to the use of assessment factors as is done in the risk assessment).

Therefore, questions to be answered here are:

1. what are the minimum data requirements to estimate the environmental improvement of a policy measure on chemicals at sufficient level of accuracy;
2. how should uncertainties be dealt with in an environmental impact assessment of chemicals.

Ad 1. This question was already answered above. With regard to uncertainty, it is noted that lack of data will generally imply an increase in assumptions and estimations. Assumptions can always be taken, they will however increase the uncertainties and in general, these uncertainties will be hard to quantify.
The HBCDD case nicely illustrates the issue of lack of data on alternatives and the assumptions that have been made to overcome the lack of data. For this case, the question where to draw the line in making assumptions to overcome the lack of data could (and should) be asked. As the alternatives to HBCDD are very uncertain, one could question the ‘real-life value’ of the impact estimates of the Policy Scenarios and thus the overall results of the study. The question whether to continue, perform further data collection or stop the assessment is case-specific and might not only be scientific, but can also be political (e.g., in case of restrictions, one could question how industry interprets the decision to stop or, conversely, continue the assessment).
Ad 2. The methodology involves a framework to deal with uncertainties including an exploratory sensitivity analysis to identify the main sources of uncertainty

and the work out of uncertainties in a quantitative or qualitative manner using existing methods for sensitivity and uncertainty analysis. A standard uncertainty table was developed to help identify sources of uncertainty and give a format to discuss the potential impacts of the uncertainties to the end results. The main aim of this framework is to provide a structure that forces (and helps) the assessor to structurally deal with all the relevant sources of uncertainty that are connected to the various steps of the impact assessment. However, the framework will not tell exactly how to assess specific sources of uncertainty (what should and can be done quantitatively and what can be done qualitatively?) and leaves the decision on the actual work to be carried out in the uncertainty analysis to the assessor. One could say that, if possible, uncertainties should be assessed in a quantitative way as this gives a more accurate estimation of the uncertainties and their impact on the results. It was also recognized that some uncertainties are difficult to capture, e.g., scenario and model uncertainties. However, the question is not only what can be done with the available data, but also, what workload is proportionate in terms of required input and obtained output of the assessment. For the case on nonylphenol, for example, it was concluded that a more detailed quantitative uncertainty analysis in terms of probabilistic exposure distributions would not change the conclusions, and therefore that the extra workload would not be proportionate to the accuracy of the output.

<u>Usefulness for policy report</u>
The added value of EIA compared to risk assessment is, firstly, the comparability of the impact results of different scenarios. The methodology introduces relative impact estimates of BAU and PS that can be compared in order to conclude whether the policy measure yields an environmental improvement and gives an indication of the level of improvement of the policy measure compared to the Business As Usual situation. Comparison of the RCR values and impact estimates as calculated in the different case studies show that RCRs alone do not tell the full story. In the nonylphenol case, RCRs of the BAU scenario show risks for the water and soil (sediment) compartments. However, the impact estimates are very low and the impact for sediment is smaller than the impact for water, despite the RCRs showing the opposite in terms of risk. Comparing the RCR and impact estimates of the nonylphenol and the zinc case, shows that the RCR values (for both cases: around 2) are not connected on the order of the estimated impact (for nonylphenol around <1% and for zinc around 15%). This is a known consequence of using a linear ‘model’ for calculating RCRs (an RCR is linearly dependent on increasing exposure concentration) while the refined impact assessment methods account for the non-linearity of SSDs and the differences in SSD slopes amongst compounds.
Depending on the actual input data and impact assessment method used, the end result has a greater or lesser absolute value. The probabilistic impact estimate comes closest to the real-life situation and the PBT ranking method gives a purely relative score with lower connection to real-life impacts. In the context of the socio-economic analysis a ‘relative’ impact estimate might not be sufficient for it to be compared with other socio-economic impacts estimates. Putting the results in the context of the case study might help understand the absolute value of the end results and might increase its value as input for the socio-economic analysis. In spite of difficulties in the application of the method, the methodology framework can minimally serve as a consistent and transparent approach to compare chemicals, especially in more complicated cases where the pros and cons of the BAU and PS scenarios are not immediately clear. This framework value increases when the methodology is expanded with other

impact and (economic) valuation modules that widen the scope of the assessment towards a full socio-economic analysis.

5.3 Follow-up

Testing of the methodology on more cases

The methodology described in this project has been developed and tested with the help of the three different case studies that are detailed in the appendices of this report. The case studies were chosen to represent a range in cases that may occur in the practice of REACH restriction (or authorisation) dossiers. However, three case studies constitute a very limited amount that also represents a limited number of possible actual situations. The case studies all showed a fairly easy conclusion with regard to comparing BAU and PS. For example, it did not present the situation at hand, in which the impact estimate of the BAU shows a high PBT score and a low impact estimate and where the PS shows a low PBT score and a high impact estimate. The methodology briefly describes what could be done in cases of comparing different types of impacts (comparing apples and oranges). As a result, however, this aspect of the methodology was not tested in an actual case study. This also ties in with the further expansion of the methodology with other impact modules, described in the next section, as then more different types of impacts need to be valued and weighed. Further testing of the methodology on actual or illustrative cases is thus required to improve and refine the methodological framework and to better understand and test the meaning of the end results. Another specific aspect of the methodology that should be further tested in practice, is the T score as part of the PBT ranking, as this equation was not part of the original POP and PBT ranking instrument developed by Rorije et al. (2011) and was therefore not extensively tested before.

Note that the case studies were performed partly parallel with the methodology, to enable two-sided learning (cases help improve the methodology and the improved methodology serves the case study progress). As a result, however, the latest adaptations to the design of the methodology were not fully worked through in the case studies (e.g., with regard to the uncertainty analysis), this is another argument to further test the methodology in other possible case studies (might be real-life or illustrative case studies).

Expansion of the methodology with additional modules

For this study, we consciously chose to focus on the methodology development of *environmental* impact assessment of chemicals. In a socio-economic analysis, however, other impact categories, such as human health impacts and other non ecotoxicity driven environmental impact categories (as in LCA) can also be relevant to estimate the socio-economic benefits of the policy measure. Expansion of the methodology with additional impact modules is thus required for SEA, and the framework was also designed to enable expansion with other impact modules. As toxic characteristics of chemicals are the main driver to start the restriction or authorisation procedure, these should in our view always be included as foreground impacts in the socio-economic analysis. However, other environmental impact categories, such as resources depletion, climate change, etc., might also be relevant in some cases and could be included as background impacts. For example, in the zinc case where the original gutter system made of zinc fundamentally differs from the alternative system made of PVC; or in the case of flame retardant HBDCC in EPS if replaced by an alternative insulation material not containing any flame retardant substance (PS3). These other background environmental impact categories could be added to the assessment

fairly easily by using standard Life Cycle impact Assessment methods, such as the ReCiPe method, part of which was used in step 4c (Goedkoop et al., 2009). Moreover, (economic) valuation modules and modules to describe impacts on markets and society could potentially be added to come to a full socio-economic analysis.
For the economic valuation of environmental impacts, the willingness to pay and ecosystem services should be further explored.

Verification

Verification of the results in actual practice of impacts on ecosystems would be valuable to check the correctness of modelled results in actual practice. For the NP/E case, verification of modelled exposure estimates was done briefly by comparing it to actual measurements. However, verification of environmental impacts will be hard in practice, as impacts on the environment are a result of a number of factors, including (a mixture of) chemicals. Estimates of environmental improvement will generally be made and used as a decision supporting instrument before the policy measure is implemented, and verification to practice is thus not possible. Verification afterwards would, however, be valuable to get a better feel for the value of these (SEA) types of decision supporting instruments.

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Abbreviations

ABS	Acrylonitrile-Butadiene-Styrene plastic
AE	Alcohol Ethoxylate
BAF	Bioaccumulation Factor
BAU	Business As Usual scenario
BCF	Bio Concentration Factor
BMF	Bio Magnification Factor
CaZn	CalciumZinc
CF	Characterization Factor
DALYS	Disability-Adjusted Life-Year
DEHP	Bis(2-ethylhexyl) phthalate
E	Effect factor
EC10	Effect Concentration 10%
ECD	Exposure Concentration Distribution
ECETOC TRA	Targeted Risk Assessment tool of the chemical trade association ECETOC
ECHA	European Chemical Agency
ECOSAR	Ecological Structure Activity Relationship
EIA	Environmental Impact Assessment
EPS	Expanded PolyStyrene
ERC	Environmental Release Categories
ESD	Emission Scenario Document
ETX programme	Computer programme to perform an SSD risk analysis based on available toxicity data
EU	European Union
F	Fate factor
FET	Freshwater EcoToxicity
HBCDD	Hexabromocyclododecane
HC50	Hazard Concentration for 50% of species
HLB	Hydrophilic-Lipophilic Balance
HIPS	High Impact Polystyrene
IS	impact score
Koa	Octanol/air partition coefficient
Kow	Octanol/water partition coefficient
LCA	Life Cycle Assessment
LCIA	Life Cycle Impact Assessment
L(E)C50	Lethal (Effect) Concentration 50% (median)
LRTP	Long Range Transport Potential
MAC	Maximum Allowable Concentration
MET	Marinewater EcoToxicity
NOEC	No Observed Effect Concentration
NP	NonylPhenol
NPE	NonylPhenol Ethoxylate
(ms)PAF	multi-substance Potentially Affected fraction of Species (for a mixture of multiple substances)
PBT	Persistent Bioaccumulative Toxic chemical
PDF	Potentially Disappeared fraction of Species
PEC	Predicted Environmental Concentration
PNEC	Predicted No Effect Concentration
PS	Policy Scenario
POP	Persistent Organic Pollutant
Pov	Overall Persistence
PVC	PolyVinylChoride

Pvap	Vapour pressure
QSAR	Quantitative Structure-Activity Relationship
RA	Risk Assessment
RAR	Risk Assessment Report
RCR	Risk Characterization Ratio
REACH	Registration, Evaluation, Authorisation and restriction of Chemicals
RIVM	Dutch National Institute For Public Health and the Environment
RHO_{susp}	Bulk density of wet suspended water
SEA	Socio-Economic Analysis
Sol	Water solubility
SpERC	Sector sPecific Environmental Release Categories
SSD	Species Sensitivity Distribution
TBBPA	Tetrabromobisphenol A
TBECH	1,2-dibromo-4-(1,2-dibromoethyl)cyclohexane
TCEP	Tris(2-carboxyethyl)phosphine
TET	Terrestrial EcoToxicity
TI	Toxic Impact
TMF	Trophic Magnification Factor
TMoA	Toxic Mode of Action
Tox	Ecotoxicity
TU	Toxic Unit
USES-LCA	The European Uniform System for the Evaluation of Substances adapted for LCA purposes
vPvB	very Persistent very Bioaccumulative substance
WWTP	Waste Water Treatment Plant
ww	wet weight

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Appendix A: Practical guidance of the methodology

The practical guidance below gives a description and explanation of the required actions to help one develop an environmental impact assessment of a chemical substance of concern compared to possible alternatives.

1.1 Step 1: Scope and scenario definition

A. Substance of concern, alternatives and first data collection: define the substance of concern, its application(s), possible alternatives and perform a first data collection on these substances. If possible, put the information in its market and societal context (what market sectors are included, who are the consumers of the products, what percentage of the total use/production of the substance is used for this application, etc.). It is also important to provide the first general information on the hazard characteristics of the substance of concern and its alternative(s) (e.g., in terms RCRs if available) and the environmental compartments of concern.

B: Decide whether environmental impact assessment of the substance of concern and its alternative(s) is possible and appropriate, based on:
- Relevance: there will be cases for which no EIA is possible, for example, because of the *lack of available data* for which EIA is not relevant, e.g., because environmental harm is not the main driver for the policy measure under study.
- Data availability: if not enough data on the substance of concern are available, it might not be possible to complete the impact assessment. However, as the reason to start this assessment is a concern for the hazardousness of a substance, it is assumed that a minimum set of data will always be available. However, the availability of data on the alternative might be more problematic, and data availability would then usually be lower than for the substance of concern. In many cases, this can be solved by taking (worst case) assumptions (resulting in higher uncertainties). However, if data availability is very limited, one could also decide to collect more data, e.g., by pursuing/asking industry or other stakeholders to provide more data, and this might imply a (temporary) stop of the impact assessment process. It is not possible to define absolute minimum data requirements for the substance of concern and its alternatives. This needs to be decided on the basis of expert judgement.
- The relevance of ecotoxic environmental impact of the substance of concern and its alternative(s): when no harmful effects to the environment (to all environmental compartments including exposure via secondary poisoning) are expected at this point in time for either the substance of concern or the alternative substance(s), there is no need to do an environmental impact assessment. This decision can be made using RCRs, if these are readily available. The cut-off RCR can be set around 1, the primary indicator for risk. If no risk indicators are available, one can base the decision whether or not an environmental impact can be expected on the available hazard data (expert judgement). When no risk to the environment is indicated by RCRs, or when available hazard data do not show harm to the environment for either the substance of concern or the alternative(s), the environmental impact assessment procedure stops here.

C. Choices and assumptions: for both the BAU and PS, choices need to be made regarding the time period, geographical scale and environmental endpoints to

serve as guides. Besides that, limited data availability will give the need to make assumptions on, e.g., trends in future production/uses, production sites, etc.
- Define the substance and the application(s) that cause concern and the main alternative(s) of the substance that provide(s) the same functionality. Depending on the case at hand, many possible alternatives can be available/under consideration. Since it would be impossible to include all alternatives in the impact assessment, one or a range (min. and max., e.g., in terms of hazardous effects) of representative alternative(s) need(s) to be chosen. Note that there are different reasons to decide whether to include a specific alternative: if possible, one should always include the alternative that is assumed to take over the functionality of the restricted substance (e.g., because of effectiveness or low costs). Other reasons to include alternatives are the (assumed) high or low environmental impact of the alternative, the high data availability for the alternative, etc.
- Define the 'replacement ratio' of the substance of concern and its alternative(s). To do this, one needs to ask the question how much (kg) of the alternative needs to be used to effectively replace the substance of concern. If no information is available on the replacement ratio one should assume a variety of ratios to investigate the effect of that on the end results (sensitivity analysis).
- Define the life cycle stages of the substance of concern and its alternative(s) that will be included in the assessment (production, formulation, processing, usage and waste stage). The starting point is to include all relevant life cycle stages and to take a similar approach for all included scenarios. If life cycle stages that might be relevant are excluded from the assessment, this should be clearly noted in the uncertainty analysis, see step 5 of the methodology.
- Define the used geographical scale of the study. As REACH is the starting point for this methodology, in general Europe or the European Union will be taken as the geographical scale of the assessment both for the scope of the restriction and for the impacts assessment. One could deviate from this on the basis of good arguments (for example, when data availability is a serious problem and only data for the Netherlands are available).
- Define the starting point in time for the policy measure and a specific time period during which the policy measure and the environmental impact are reviewed. A careful definition of the included time period is important, for the life cycle of the product will have a certain time span (product lifetime), exposure of the substances will take time and the environmental impacts will probably occur in the years following exposure. The latter (exposure-effect delay) will generally not be accounted for, as hazard data will not give this information.
- Define the critical toxic/adverse environmental effects of the substances of concern and the alternatives, as well as the relevant environmental compartments (water, sediment, soil, air, secondary poisoning). In some cases, this may result in the choice to perform a more targeted EIA (for example, for the water compartment only). If such a limited scope is chosen, other possible/expected environmental effects caused by ecotoxicity need to be written down as PM, so that a complete overview of possible/expected impacts will be obtained qualitatively. Also if other than ecotoxicity environmental endpoints (climate change, resource depletion, human health impact etc.) are thought to be relevant, they must be written down as PM for a complete overview of possible impacts and possible latter extension of the impact assessment. Note that if one of the substances of BAU and PS is presumed to be PBT, secondary poisoning should always be included as a relevant environmental assessment approach.

D. Define the Business As Usual (BAU) scenario: representing the situation in which the production/use/placing on the market of the substance of concern in its (various) application(s) is continued. Here, define European production and use volumes including import and export volumes if relevant depending on the actual restriction as defined in the Policy Scenario (i.e., a restriction on use will affect import, and a restriction on production will affect export). Other measures or situations affecting the future production/use volumes of the substance (market trends, without a restriction) that have already been implemented should be taken into account wherever possible.

E. Define the Policy Scenario(s) (PS): representing the situation in which manufacturing, placing on the market and/or usage of the substance of concern in application(s) are restricted. This includes the substance(s), application(s), the effective date, and optionally the maximum allowed concentration of the substance and optional derogations (e.g., in time or for a substance in a specific application). If relevant, variations of the restriction can be included (PS1, PS2, etc.).
For a complete representation of the environmental impacts, two steps need to be taken:
- Quantify the reduction in production/use volume of the substance of concern after the restriction. In case of a full restriction we may assume that volumes (and thus emissions) for that application go to zero as soon as the restriction enters into force.
- The restriction on the substance of concern means that the function of the substance needs to be provided by an alternative substance(s) (or in an alternative manner). The production/usage volume of the alternative substance(s) nee(d) to be part of the Policy Scenario. In defining the production/use volume, the replacement ratio of the alternative substance needs to be taken into account. (Be aware that this does not automatically mean that the volume of substance of concern and alternative substances are comparable as the alternative substances can be more/less effective.)

Note: the choices and assumptions made in this step need to be included in an uncertainty table to keep track of sources of uncertainty that might influence the end result of the assessment. See the description on dealing with uncertainties in step 5.

1.2 Step 2: Exposure and hazard estimation

Tiered approach

A: The quality and level of detail of the assessment at first depends on the data availability. If data availability is limited, it will only be possible to do the assessment with low specificity, with lower tier methods.
B: If more data are available, the quality and level of detail of the assessment are determined based on what is proportionate to come to an end result: estimate the environmental improvement of introducing the policy measure (PS minus BAU). In cases where the difference in environmental impact between BAU and PS is not so obvious and in cases where the certainty of BAU or PS differs (first indication of different levels of uncertainty) a higher tier of assessment methods needs to be chosen, including the quantitative assessment of uncertainty.
C: For the sake of comparability applying the same level of detail for BAU and PS is recommended.

Step 2a. Release estimation

A: The specific application of both the substance of concern and the alternative have been determined and described in the previous step. The next action is to *collect data on actual or estimated releases or release factors* for all life cycle stages of the substance of concern and its alternative(s) and to select the most relevant release factors for the case under study. If this data set is not available, the relevant or representative ESD or SpERC has to be selected for both the BAU and Policy Scenarios, so that release estimates can be deduced from this document. Within an ESD, several sub-scenarios of the production or use of the substance may be available. If this is the case, the most common or most relevant scenario (by volume) for both the substance of concern and the alternative needs to be selected based on the BAU and Policy Scenarios defined earlier. Note that ESDs usually provide worst case release factors. Sometimes, however, realistic case factors or ranges of release determining parameters are available as well. Within the context of an impact assessment, a realistic assessment is more favourable than a worst case assumption. When release factors are very uncertain, one could vary the release factors to determine the sensitivity to the end results. Further information on use and scope of ESDs and their applicability can be found on the OECD website[2].

B: Determine the *relevant life cycle stages* for the substance of concern and the alternative(s). Depending on the source of release information (ESD or other) the focus of the release estimation may be on each of the relevant life cycle stages, or only on the most relevant life cycle stage in terms of release and exposure. Which life cycle stages to include thus depends on the data availability and the way the restriction is defined (e.g., total ban on production and use, only a ban on a specific use etc). When not all relevant life cycle stages could be included, this should be explicitly stated in the assessment report.

C: Estimate for both the BAU scenario (substance of concern) and the PS (alternative substance) the *releases to all relevant environmental compartments* (air, water, sediment and soil) based on all relevant life cycle stages. This can be achieved by combining the release factors with the production/use volumes as defined in step 1. Note that one should include volumes of the substance of concern (BAU) and the alternative(s) (PS) based on the replacement ratio as defined in step 1.

Table 7: Data requirements release estimation

Minimum quality (low tier)	**Preferred quality** (high tier)
For the selection of the right ESD/(Sp)ERC: - Amount used in a Region (country) or in the European Union (continent) - Use description - Life cycle stages - Content of the substance in the preparation or in the article *For the calculation of release factors* - Physical and chemical properties (vapour pressure, water solubility, octanol-water partition coefficient)	- Actual release information for air, water and soil for all relevant life cycle stages *Depending on the actual form of the available release information, additional information might be required:* - Amount used in a Region (country) or in the European Union (continent) - Use description - Life cycle stages - Content of the substance in the preparation or in the article

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[2] http://www.oecd.org/document/46/0,3746,en_2649_34379_2412462_1_1_1_1,00.html

Note that, for the minimum quality assessment, the actual required data can be very different based on the ESD/(Sp)ERC used. If the information cannot be easily retrieved, the default values provided in the ESD can be used, but this is not preferred, as the scenarios are not discerning enough with respect to releases.

Step 2b. Exposure estimation

A: In order to perform the calculations in EUSES, the physical and chemical properties and data on the biodegradability of the substance have to be known and used as input. In view of considering uncertainties in the environmental impact assessment, the uncertainties in the physical and chemical properties and biodegradability should also be taken into account. The degree of uncertainty can be estimated by gathering as many data as possible on the basis of measurements. Alternatively, standard uncertainty distribution functions can be applied. These distribution functions have been derived from Hollander et al. (2011) for the basic set of substance properties needed in the environmental exposure assessment. The following data are essential for the fate calculations:

Table 8a: Data requirements exposure estimation (1)

Minimum quality (low tier)	**Preferred quality** (high tier)
Based on EUSES - Molecular weight - Water solubility - Vapour Pressure - Melting point - Boiling point - Octanol-water partition coefficient - Information on the chemical class for the application of the QSAR for bioconcentration factors. - Data on the biodegradability of the substance, either half-lives in the various compartments or results from standard biodegradability tests as defined in the EUSES model. - If available quantitative/qualitative information on the uncertainty of the used input parameters	Based on EUSES - Molecular weight - Water solubility - Vapour Pressure - Melting point - Boiling point - Octanol-water partition coefficient - Information on the chemical class for the application of the QSAR for bioconcentration factors. - Data on the biodegradability of the substance, either half-lives in the various compartments or results from standard biodegradability tests as defined in the EUSES model. - Quantitative information on the uncertainty of the used input parameters (estimated on the basis of measurement data or on standard distribution functions)

B: Next, the releases to the various environmental compartments calculated in step 2a have to be entered in the EUSES fate model. The releases can be entered for each relevant life cycle stage considered in the environmental impact assessment, in order to calculate the impact for each life cycle stage separately. In addition, a calculation based on the total release can be performed to estimate the total impact per environmental compartment at the regional (country) or continental (EU) scale. For a detailed analysis, the environmental impact on the local scale should also be estimated for each relevant life cycle stage. A local impact assessment, however, often requires additional data with respect to the regional or continental assessment. It is, therefore, recommended to first perform a regional assessment. If there are no risks identified at the regional scale, a local impact assessment has to be performed to identify the life cycle stage and uses of concern. This step will result in Predicted Environmental Concentrations (PECs) for all (relevant or available) environmental compartments and the sewage treatment plant.

Table 8b: Data requirements exposure estimation (2)

Minimum quality (low tier)	**Preferred quality** (high tier)
Calculation in EUSES Include all available life cycle stages* Include all available environmental compartments* Calculation at regional and continental scale, if relevant and possible also at local scale	Calculation in EUSES Include all (relevant) life cycle stages Include all (relevant) environmental compartments Calculation at regional and continental scale, if relevant also at local scale

***** *When life cycle stages or environmental compartments that are assumed to be relevant are excluded from the assessment, this needs to be stated explicitly.*

Step 2c: Hazard assessment

A: Retrieve toxicity data, acute or chronic, for at least three different taxonomic groups of aquatic, soil or sediment organisms. Furthermore, a NOEC, EC_{10} or EC_{50} from a growth or respiration inhibition test for microorganisms is needed. If availability of hazard data is very limited, additional data could be derived using QSAR of ECOSAR models (EPISuite 4.0, 2009). These models can also be used to evaluate or check hazard information provided by experimental studies using the Weight of Evidence method.

B: PNECs need to be derived through the application of default extrapolation factors on the single species toxicity data. Default extrapolation factors can be replaced by substance-specific or database-derived factors, if available.

C: Determine the environmental compartments, ecosystems or species potentially at risk. These are the compartments where environmental impacts may be expected. Qualitatively describe the mechanism that will cause the effect. Other potentially harmful characteristics of the substance (persistence, bioaccumulation, long range transport potential…) should also be listed.

D: Decide for what risks and hazard characteristics potential harmful environmental impacts can be derived in the next step.

Table 9: Data requirements and outputs hazard assessment

Minimum quality (low tier)	**Preferred quality** (high tier)
For all available or relevant environmental compartments	*For all relevant environmental compartments*
- L(E)C_{50} for fish, daphnia and algae	- L(E)C_{50} for fish, algae, daphnids, crustacean and other species is available - NOEC, EC_{10} or EC_{50} from a growth or respiration inhibition test for microorganisms.
- Uncertainty information to determine assessment factors.	- Uncertainty information to determine assessment factors.
- Knowledge on toxicity, persistence and bioaccumulative characteristics of the	- Knowledge on toxicity, persistence and bioaccumulative characteristics of the substance

substance of concern and the alternative and the underlying mechanisms.	of concern and the alternative and the underlying mechanisms.
- PNEC- water organisms *And more if available*	- PNEC- water organisms - PNEC-terrestrial organisms - PNEC-sediment - PNEC-micro-organisms - PNECoral birds/mammals

1.3 Step 3: Determination of endpoints and assessment method

A: Risk(s) driven by toxicity only? As illustrated in Figure 2, the question is raised whether the risk(s) is (are) driven by toxicity only, or by additional properties such as P and B (or vPvB). Determine the relevant endpoints for both the substance of concern (BAU) and the alternative substance (PS). Cases indicated to be toxicity-driven only continue to B1, cases in which (one of) the scenarios consist(s) of persistent and/or bioaccumulative substances continue in B2.

B1.Toxicity driven only: If the risks are driven by toxicity only, a deterministic (4b) or probabilistic (4c) environmental impact assessment method can be used to quantify impacts. Both methods are part of the tiered approach, and the decision on what method to choose depends on the data availability on exposure and hazard (what is possible) as well as on what is thought to be the proportional method in view of the required input and the obtained result output. One could say in general that in cases where the difference between the impact results of BAU and PS are rather obvious, a lower tier approach can be applied (4b. deterministic approach, lower tier). A higher tier approach (4c. probabilistic approach, higher tier) is chosen if differences are less obvious. The ‘semi-‘probabilistic approach using point exposure estimates can be seen as an in-between tier. It should be mentioned that the higher tier approach is preferred when results are intended to be used as input for a wider socio-economic analysis, as this will provide more realistic end results.
The question what method is proportionate can differ per case and should be decided on the basis of expert judgement. One could also decide to apply both methods to a case. Before one continues with the actual impact assessment in step 4, one first needs to estimate whether this impact assessment is as valuable as described in action C.

B2. Toxicity and PB driven: If one of the substances is indicated to be PBT or vPvB, PBT ranking needs to be assessed in any case for BAU and PS. Note that PBT ranking will *always* be applied for *both* the substance of concern *and* for the alternative, to enable the comparison between BAU and PS, even if one of the substances is not identified or potential PBT. Note that the PBT and vPvB criteria for Annex XIII to the Regulation do not apply to inorganic substances (ECHA, 2008b) and that the P and B ranking methods cannot be applied to these substances. Depending on the number of inorganic alternatives included in a study it might not be useful to perform PBT ranking, as the ranking is a comparative method. Besides the PBT ranking, a (probabilistic or deterministic) impact assessment will also be considered to get an impression of the toxicity in combination with expected releases and exposure. This impact assessment should at least include secondary poisoning as (one of the) environmental compartment(s). To decide whether or not it is useful to perform an impact assessment (4b or 4c) for the case under study, one should continue with action C before entering step 4.

C. Estimation of RCRs for both BAU and PS: For both BAU and PS, determine the RCR values for all relevant environmental compartments based on the PEC and PNEC value estimated in steps 2b and 2c. The outcome of the RCRs are used to decide whether it is relevant to continue the EIA for the case under study or whether the EIA can be stopped at this point. If all RCRs for BAU and PS are below 0.8 (or 1), the impact assessment will stop here. If one of the RCRs of BAU and PS is above 0.8 (or 1) the impact assessment will be continued. Note that this is more or less the same decision as was made in step 1 of the methodology, although by now more data on which to base the decision have been collected and processed (resulting in more realistic RCRs).

1.4 Step 4: Environmental impact assessment of chemical substances

Step 4a. PBT ranking
A. Collection of input data: Collecting experimental information on the persistency, bioaccumulation and toxicity of the substances (Pov, BAF and PNEC for the water compartment). When data on persistency and bioccumulation are not available, the data needed should be estimated on the basis of QSARs, as described by Rorije et al. (2011).

B. P, B and T scoring: Calculate the P, B and T scores based on the equations 1, 2 and 3 presented in section 1.4.1 from chapter 4 of the report.

C. Sum: Sum the results from the P, B and T scoring on a 1:1:1 basis to derive a total PBT score.

Step 4b. Environmental impact assessment based on a deterministic approach
For all relevant receiving environmental compartments *j,* collect the fate factors for the substances considered in the BAU and PS, taking into account the emission compartment *i*. Depending on the number of compartments to which the substance is emitted (*i*) a number of fate factors need to be collected per receiving environmental compartment (*j*). The fate factors can be collected from Appendices C-F published by Huijbregts (2004). If fate factors for the substances under study are not available in Huijbregts (2004) one could calculate the factor using USES-LCA 2.0. However, this requires quite some effort and expertise.

For all relevant receiving compartments (*j*), determine the effect factors of the substances considered in the BAU and PS. To determine the effect factors equation 6 can be used. To use this equation the HC50 values for water of the substances under consideration are required at least. Preferably the toxic mode of action of the substance under consideration is known to determine the change in PDF per change in toxic mode of action ($\partial PDF_{tox}/\partial TU_k$).

If the substances under consideration are emitted to several compartments (*i*), determine for each emission compartment *i* the release rate $Q_{s,i}$ in kg per year.

Determine for each emission compartment *i* and receiving compartment *j* the characterization factors $CF_{i,j,s}$ according to equation 7 or 8.

Subsequently, compute for each emission compartment *j* the impact scores, $IS_{i,j,s}$ according to equation 9. If a number of impact scores are calculated per receiving environmental compartment *j,* due to a number of different emission compartments *i* for that substance, all impact scores per receiving environmental compartment *j* need to be added up. This will result in an impact score IS for fresh water (FET), marine water (MET) and terrestrial ecosystems (TET) expressed as potentially disappeared fraction of species (per year).

Step 4c. Environmental impact assessment based on a probabilistic approach
A: Use the Excel spreadsheet model of SimpleBox in combination with Monte Carlo programmes that are compatible with this spreadsheet to calculate the (logarithmic) exposure concentration distribution. Instead of using single value input parameters in the spreadsheet of environmental fate and exposure models (as has been described in step 2b) this can be done by including distributions of the input variables. The most uncertain input variable(s) is (are) probably the emission rate(s). It is, therefore, very important to estimate the distribution of possible emission rates, for this input parameter at least. From a pragmatic point of view, this can be achieved easily by assuming, for example, an asymmetric triangle distribution of emission rates. A similar approach is probably satisfactory for parameters which are usually surrounded by high margins of uncertainty like first order (bio)degradation rates (or half-lifes). The output of the spreadsheet is a distribution of exposure concentrations in the different environmental compartments (=ECDs). If it is not possible to derive an exposure concentration distribution, one can also decide to use point exposure estimates for the different relevant environmental compartments.

B: Use the ETX programme (Van Vlaardingen et al., 2004) to calculate the environmental impact in potentially disappeared fraction of species. This can be done by introducing the ECD per environmental compartment and the available L(E)C50 data for the specific environmental compartment into the ETX programme. Note that to be able to calculate an SSD, a minimum of four or five LC50 values for different organisms is required. To obtain a realistic distribution of the species sensitivity to predators (bird, mammal, fish) for secondary poisoning three or four chronic or repro toxicity data are required at least, that can be integrated into one SSD. These can be toxicity data from the taxonomic groups bird, mammal and fish (if combination in an SSD is acceptable) or from one (of the) taxonomic group(s) (separately).
The programme will then produce a cumulative SSD function to be multiplied with the ECD. This needs to be carried out for all relevant environmental compartments. The output is the toxic impact (TI) expressed as potentially disappeared fraction of species due to exposure to a chemical substance which is present according to a certain distribution in the relevant compartment. As appropriate, the potentially disappeared fraction based on available L(E)C50 data can be replaced by a Potentially Affected Fraction at another level of test impacts, e.g., chronic EC50s, or chronic NOECS, when the exposure data (distribution) are positioned (far) left of the SSD. In doing so, the sensitivity of the BAU and PS is increased, since impact estimates now depend on the steep part of the SSD rather than on the lower tail.

1.5 Step 5: Dealing with uncertainties

A: Prepare an overview table of sources of uncertainty for the case study, including BAU and PS scenarios based on the standard uncertainty table presented in section 3.6 of the report (Table 4). Check whether all relevant sources of uncertainties for this specific case are included in the table. If not, add the case-specific sources in the overview and complete the table.

B: Perform a sensitivity analysis on the sources of uncertainty that are expressed quantitatively to estimate the relevance of the source of uncertainty for the end results. This can be achieved by variation of the parameters that are assumed to be relevant. For the qualitatively described parameters, choices and assumptions it is more difficult and should be based on expert judgement.

C: Fill out the various columns of the uncertainty table using the column descriptions below the standard table. The columns should be filled out quantitatively (level 2 or 3) whenever possible and assumed proportional. Alternatively a qualitative analysis can be used on the basis of expert judgement (level 1). One could also describe a relevant source of uncertainty both quantitatively and qualitatively if this helps to get a better impression of the source of uncertainty.

Note that actions A, B and C will partly be performed in parallel, as it is hard to indicate all the relevant sources of uncertainty and to perform a sensitivity analysis if one does not have an overview of the input parameters used. On the other hand the outcome of the sensitivity analysis will help to determine the proportionate level to fill out the uncertainty table.

D: Prioritize and rank the various sources of uncertainties (both the quantitatively and qualitatively described uncertainties) by indicating the major sources for this case study. The major sources of uncertainty can be highlighted in **bold** and ranked in order of importance. This action is in line with action D (criteria and scaling evaluation) as described on page 17 of the uncertainty analysis guidance of ECHA (ECHA, 2008c). Since it will not be possible to rank both the quantitative and qualitative sources in one ranking list, this action can result in a qualitative as well as a quantitative list.

E: Estimate the overall influence of the uncertainties on the end results. Do the uncertainties affect the possibility to conclude on the difference in environmental impact of BAU and PS? Are the uncertainties likely to cause an overall over- or underestimation? For some sources of uncertainty, it will not be possible to estimate the influence on the end result. The uncertainty could mean an over or underestimation. However, the importance of this uncertainty is not known, nor is the influence on the end result. This should also be stated.

F: If major sources of uncertainties that could be reduced have been identified, e.g., by increased data collection, this should be stated including suggestions for improvement that could be taken to improve the certainty of the end result.

G: To increase the reliability (and reduce the subjectivity) of the uncertainty analysis, the above actions, based on expert judgement, should be performed individually by a number of different experts. The experts can do this on the basis of the text description of the case study and by means of an empty uncertainty table (only the quantitatively described uncertainties can be filled out). After a number of experts have filled out the table , they come together and discuss the uncertainty sources based on the different uncertainty tables. The goal of the discussion is to create one final uncertainty table that all experts agree on. When experts disagree on aspects of the table, both views will be included in the final uncertainty table.

1.6 Step 6: Comparison of the scenarios

A. Comparison of PBT scores, probabilistic and deterministic impact estimates (and/or RCRs):
Firstly, compare the estimated impacts BAU and PS for all applied impact assessment methods individually. Per impact method one needs to estimate the impact difference by subtracting BAU from PS. (PS minus BAU gives the impact gain of applying the Policy Scenario). The difference can also be estimated by dividing BAU by PS (PS : BAU gives the 'level of improvement'). Drawback of the latter method is that at very low impact estimates, the level of improvement can be very high, while the absolute improvement is only marginal.

B. Combination of impact estimates: If different impact assessment methods are applied, make a combination of the impact estimates as described in section 3.7 of the report. This should help to come to a conclusion on the environmental improvement of introducing the Policy Scenario compared to the Business As Usual situation.

C. Uncertainties in results: Step 5 gives an indication of the uncertainties and the possible effect of this on the end result. The most relevant uncertainties should be explained in the results and – if possible – an indication of the effect of the uncertainties on the end results should be given. Always indicate whether the difference is significant (either quantitatively of qualitatively).

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Appendix B: Nonylphenol and nonylphenol ethoxylates in detergent applications replaced by alcohol ethoxylates, an historic case study

1.1 Step 1: Scope and scenario definition

1.1.1 Description of the case

Nonylphenol (NP) is on the second priority list of substances drawn up under the European Union's Existing Substances Regulation (793/93/EEC). NP is on this list due to the large quantity produced and used annually, its toxicity to aquatic organisms, and concerns that it is not readily biodegradable. Furthermore, NP is classified as an endocrine disruptive compound, displaying some estrogenic activity.

A European environmental risk assessment (RAR) for nonylphenols (NP) and their ethoxylates (NPE) (EC 2002) indicated the need to reduce risks associated with their production, their formulation into other products and the end use of these products in a wide range of industries.

The risk assessment report (RAR) concluded that aquatic, terrestrial and secondary poisoning (e.g., bioaccumulation) risks were unacceptable. In terms of lowest observable effect levels (LOEL), the most sensitive of these 'endpoints' is the aquatic environment. Nevertheless, the risk reduction strategy must be designed to deal with each of these endpoints effectively. Next to general toxicity, other criteria, such as endocrine disruption, should also be evaluated in the design of the risk reduction strategy.

The background regional predicted environmental concentration for water (PEC_{water}) is calculated to be 0.6 microgrammes per litre (µg/L) for the year 1997, while the predicted no effects concentration for water ($PNEC_{water}$) is calculated to be 0.33 µg/L, based on a chronic algal toxicity test (*Scenedesmus subspicatus*) with a 72 hr EC_{10} of 3.3 µg/L (Kopf 1997) using an assessment factor.

Actual historical case
As early as in 1999, an early first proposal for a risk reduction strategy was commissioned by the UK Department of the Environment, Transport and the Regions (RPA 1999). A mix of policy measures is recommended to address the environmental risks associated with NP and NPE (NP/E).

By Directive 2003/53/EC of the European Parliament of 18 June 2003, the EU largely adopted the UK risk reduction strategy to be implemented by the member states as from 17 January 2005. The following restriction entry was added to the Council Directive 76/769/EEC, relating to restrictions on the marketing and use of certain dangerous substances and preparations:

'Nonylphenol and Nonylphenol ethoxylates may not be placed on the market or used as a substance or constituent of preparations in concentrations equal or higher than 0,1 % by mass for the following purposes:

1. industrial and institutional cleaning except:
   - controlled closed dry cleaning systems where the washing liquid is recycled or incinerated,

   - cleaning systems with special treatment where the washing liquid is recycled or incinerated;
2. domestic cleaning;
3. textiles and leather processing except:
   - processing with no release into waste water,
   - systems with special treatment where the process water is pretreated to remove the organic fraction completely prior to biological waste water treatment (degreasing of sheepskin);
4. emulsifier in agricultural teat dips;
5. metal working except:
   - uses in controlled closed systems where the washing liquid is recycled or incinerated;
6. manufacturing of pulp and paper;
7. cosmetic products;
8. other personal care products except:
   - spermicides;
9. co-formulants in pesticides and biocides.’

In summary, the restrictions are mainly related to the detergent properties of NPEs as applied in industrial, institutional and domestic cleaning, textiles, leathers, agriculture (veterinary medicines), metals, pulp and paper, and cosmetics. Upon release, NPE is quickly converted to NP, which is not readily biodegradable. It is believed that the measure to restrict the use and marketing of highly concentrated NPE as a detergent would eliminate some 70% of the NP burden, reducing the background regional concentrations to below 0.18 µg/L and thus below the PNEC of 0.33 µg/l.

In this case study, the ecotox environmental impact of this historic restriction will be assessed.

Substitutes for NPEs

In the Directive 2003/53/EC, the EU did not prescribe the use of alternative substances.

In developing a risk reduction strategy, it is, however, important not only to take into account the results of the risk reduction by phasing out a particular compound, but also to address to the extent possible any new risks (and impacts) which may result from the use of substitute chemicals and/or other changes (e.g., alternative processes or techniques) brought on by implementing the strategy.

In the case of NPEs, many industries noted that various alcohol ethoxylates (AE) are primary substitutes and that these pose a lesser risk to the environment than NPEs (RPA 1999; ToxEcology 2002). It must be recognized that the categories ‘NP’ and ‘NPE’ represent a significant number of different chemicals. NPs may be either branched or straight chain molecules. In addition to these variations, NPEs may have differing degrees of substitution by ethylene oxide. Furthermore, the extent of ethylene oxide polymerisation and nature of chain branching will vary between molecules within a particular formulation. The term alcohol ethoxylates thus represents a yet wider group of chemicals. Not only may the degree of ethoxylation vary, but the chain length of the parent alcohol may vary as well (although this is generally not significant within individual formulations). Depending on the exact structure, the toxicity of both NP/Es and AEs varies considerably. Since specific information regarding precisely which chemicals are used in case of NPEs - or could be used in case of AEs - is not available, accurate comparisons of risk and impact scenarios cannot be made.

By far the most common replacement for NPEs are AEs. Based on available data, the following conclusions were drawn comparing NPEs and AEs (ToxEcology 2002):

- The intact surfactants, AE and NPE, exhibit a similar range of toxicity to aquatic organisms
- Removal rates for the parent surfactants in waste water treatment plants (WWTP) are similar for AE and NPE, since both vary depending on the type of WWTP and operating conditions and both can be >90% when subjected to treatment in well-functioning WWTP
- AE are readily and ultimately biodegradable
- NPE are ultimately but not readily biodegradable
- The biodegradation intermediates of AE are less toxic than the parent surfactants
- The biodegradation intermediates of NPE (specifically NP) are more toxic than the parent surfactants
- None of the AE compounds is endocrine disruptive, unlike NP
- The average predicted no-effect concentration for a commonly used commercial AE (C13.3 EO8.2) has been estimated to be 110µg/L: (Van de Plassche et al. 1999).
- The PNEC for NP is 0.33 µg/L (EC 2002)
- Recent risk assessments on AE (HERA 2009 (version 2)) (which take into account the higher uses of AE in recent years, since they have been used as substitutes for NPE in Europe) indicate a reasonable margin of safety and low concern for the aquatic environment

1.1.2 *Scenario definition*

The scenarios assessed in this case study describe the situation in which no policy action is taken on the European level to address the risks of the use of NP/E (BAU), compared to the scenario in which the restriction of NP/E as presented above entered into force from 2005 onwards (PS).

Business As Usual scenario
In the BAU scenario, the 1997 production and use volume of NP/E in Europe is considered to continue unchanged up to the year 2005. Similarly, the 1999 use of AE is considered to be unchanged up to the year 2005. The 1997 use volume of AE is considered to be equal to the AE use volume in the year 1999.

Nonylphenol and nonylphenol ethoxylate
The 1997 use of nonylphenol is presented in Figure 5 (EC 2002). The 47,000 tonnes of NP used for the European NPE production results in an quantity of 118,000 tonnes of NPE. Of this quantity, 77,600 tonnes of NPE are actually used in the EU.

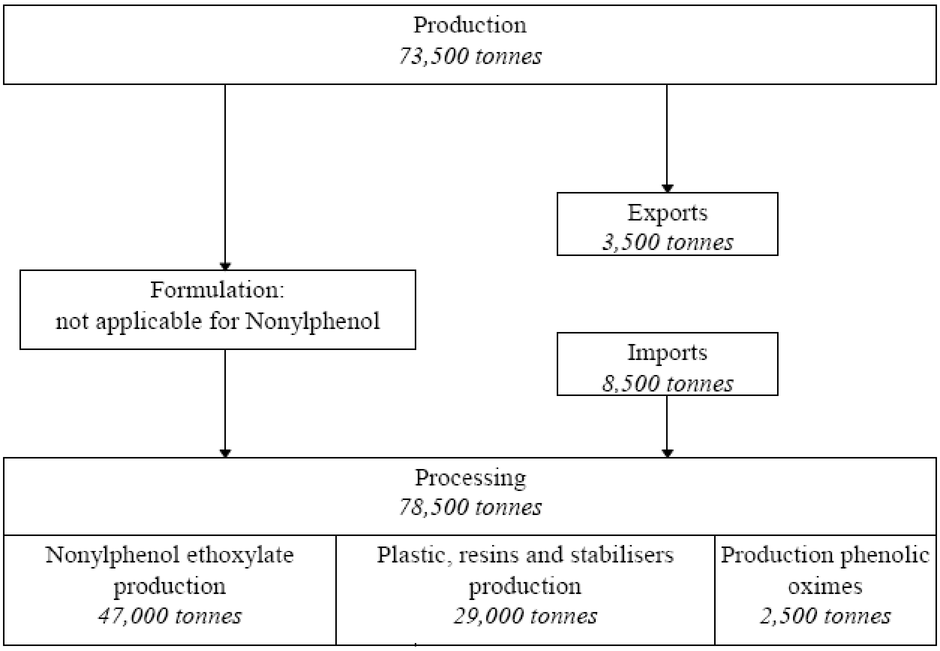

Figure 5: Nonylphenol lifecycle (all figures refer to the quantity of nonylphenol, 1997)

Alcohol ethoxylates
In 1999, a survey of AE producers reported that approximately 290,000 tonnes of AE were thought to be used in Europe as detergents for household cleaning products (HERA 2009 (version 2)). This amount is included to calculate the (background) concentrations of AE in the BAU scenario.

<u>Policy Scenario</u>
In the Policy Scenario, the detergent use of NPE is restricted as described in the legal text above. The restriction of the detergent use of NPE is considered to be compensated in the market by completely replacing the detergent use of NPE by the use of a variety of AE homologues, and not by other kinds of detergents.

Although the toxicity of AE to aquatic organisms is compound- and species-specific, several generalizations concerning chemical structure and toxicity are made based on the available data (ToxEcology 2002):

- Toxicity generally decreases with increasing EO chain length
- Toxicity generally increases as alkyl chain length increases
- Branched alkyl chains are less toxic than linear alkyl chains
- Secondary attachment of the alcohols reduces toxicity compared to primary alcohols
- AE containing propylene oxide (PO) units are less toxic than those containing only EO

In our case study, C10EO3 (CAS reg. no. 68439-46-3 – description: Alcohols, C9-11, ethoxylated) has arbitrarily been chosen as the representative AE, because this group of AEs has similar technical characteristics in a comparison of NPE and AE based on standard scales and measures of surfactant properties and use applicability (ToxEcology 2002, Tables 20, 21 and 22). Surfactants are generally compared on the basis of a number of physico-chemical characteristics. For ethoxylated surfactants, such as AE and NPE, general detergent efficacy comparison considered aspects as alkyl chain length and range and degree of ethoxylation, physical appearance at 25 ºC (e.g., liquid/solid), molecular weight, melting point, freezing point, colour, specific gravity, viscosity, hydroxyl number, flash point, cloud point, pour point, and Hydrophilic-Lipophilic Balance (HLB) values. Furthermore, this choice has been guided by considerations on the distribution of toxicity (not the most toxic, but also not the least toxic) and degradability (readily degradable, like most AE homologues) of the model alternative compound.

If we assume that the average NPE has seven ethoxylate groups (NPE7) (EC 2002), this results in an average molecular mass of 528 g/mole. The AE C10EO3 has a molecular mass of 290 g/mole. If we assume equal molar detergent efficacy, an equally effective replacement of NPE by AE would require an amount of C10EO3 that is 45% lower (100%-290/528x100%) in use volume, as well as in daily emissions to WWTPs. The different replacement scenarios, however, account for a possibly different detergent efficacy of AE (sensitivity analysis).

By the year 2005, 100% of the 1997 European emission of NPE is assumed to be replaced by a variable extra emission of the AE on top of the already existing emission based on the use volume of AE in 1999 (= 1997):

- Policy replacement scenario a: On a weight-by-weight basis, an emission of AE equal to the 1997 emission of NPE is supposed to be added.
- Policy replacement scenario b: On a weight-by-weight basis, an emission of AE equal to half the 1997 emission of NPE is supposed to be added. Due to considerations of equal detergent efficacy, this is the most realistic scenario.
- Policy replacement scenario c: On a weight-by-weight basis, an emission of AE equal to double the 1997 emission of NPE is supposed to be added.

1.2 Step 2: Exposure and hazard estimation

1.2.1 Step 2a: Release estimation

Release estimation for BAU scenario

All NPE and AE used as detergent in Europe is generally released to WWTP installations as an aqueous solution (EC 2002; HERA 2009 (version 2)). In the sewer or during sewage treatment processes, some of the detergents will be adsorbed by solids, and may then undergo anaerobic biodegradation in a digester before the resulting sludge is released to agricultural land, for use as fertilizer. The detergent remaining in aqueous solution is subject to aerobic biodegradation processes during sewage treatment, which results in substantial removal before the effluent is released to surface water. In surface water, sediment and soil, further aerobic and anaerobic biodegradation will occur. The big difference between NPE and AE is the difference in the degradation rate of the parent alcohols, where the degradation of NP is much slower than the degradation of alkanols.

Nonylphenol and nonylphenol ethoxylate

According to the EU RAR for NP (EC 2002), in 1997 the European production, handling and all categories of NP/E use result in an annual average continental emission of NP to air of 946 kg/d and to surface water of 2979 kg/d. On the regional scale these emissions are 106 kg/d and 319 kg/d, respectively. For approximately 95%, the NP emissions to surface water are the result of NPE emissions to WWTP facilities. If NPE is released to a WWTP, the resultant emission of NP to surface waters is 2.5% of the NPE emission to the WWTP. In 1997, all of the continental and regional emissions of NPE (respectively 108,060 and 12,006 kg/d) are considered to be treated in a WWTP.

Alcohol ethoxylates
The 1999 continental emission of detergent AE to WWTP installations is approximately 800,000 kg/d (HERA 2009 (version 2)). In the BAU scenario, this emission is considered equal for the years 1997, 1999 and 2005.

Release estimation for Policy Scenario

Nonylphenol and nonylphenol ethoxylate
In 2005, the European restriction of the use of NP and NPE for the major use categories is believed to result in 70% reduction of the NP burden (RPA 1999) and a proportional reduction of the emissions to surface water. This results in continental and regional emissions of NPE to WWTP installations for the year 2005 of 32,419 and 3602 kg/d, respectively.

Alcohol ethoxylates
The releases of C10EO3 for the different replacement scenarios, are presented in Table 10.

Table 10: Continental and regional emissions of C10EO3 for different replacement scenarios

Policy replacement scenario	Continental emission kg/d	Regional emission kg/d
a = 50% AE ww	54,030	6003
b = 100% AE ww	108,060	12,006
c = 200% AE ww	216,120	24,012

1.2.2 *Step 2b: Exposure estimation*

Exposure estimation for BAU scenario

Nonylphenol
In 1997, the production, handling and use of NP/E leads to the following predicted environmental concentrations of NP on the regional scale (EC 2002):
- PEC_{Water}: 0.6 µg/L dissolved
- $PEC_{Sediment}$: 0.103 mg/kg wet weight
- PEC_{Soil}: 0.265 mg/kg wet weight

Alcohol ethoxylates
The alcohols used in the manufacture of AE typically contain an alkyl chain with 8 to 18 carbon atoms while the ethoxylate chain typically averages from 3 to 12 ethylene oxide units (Talmage 1994). For the year 1999 (equal to the years 1997 and 2005), the summed PEC values for all non-replacement AE uses and all AE homologues as determined for the different environmental compartments is given in Table 11 (HERA 2009 (version 2)).

Table 11: PEC values for different environmental compartments expressed as the sum for a realistic mixture of the most likely 222 AE homologues (C8-18 EO=0-22)

Environmental Compartment	PEC value for sum of AE homologues
Surface water	$PEC_{\text{local water dissolved}}$ = 1.01 µg/l
Sediment	$PEC_{\text{local sediment}}$ = 1.01 mg/kg wet weight
Soil	$PEC_{\text{local soil (30 days)}}$ = 0.24 mg/kg wet weight

Exposure estimation for PS

Nonylphenol

In 2005, the European restriction of the use of NP and NPE for the major use categories is believed to result in a 70% reduction of European environmental background concentrations of NP on a regional scale (RPA 1999):

- PEC_{Water}: 0.18 µg/L dissolved
- PEC_{Sediment}: 0.031 mg/kg wet weight
- PEC_{Soil}: 0.080 mg/kg wet weight

An example of the actually observed concentration reductions of NP is presented in Figure 6 (Quednow and Püttmann 2009). These data imply a reduction of NP concentrations that are even less than 70% of the 1997 situation.

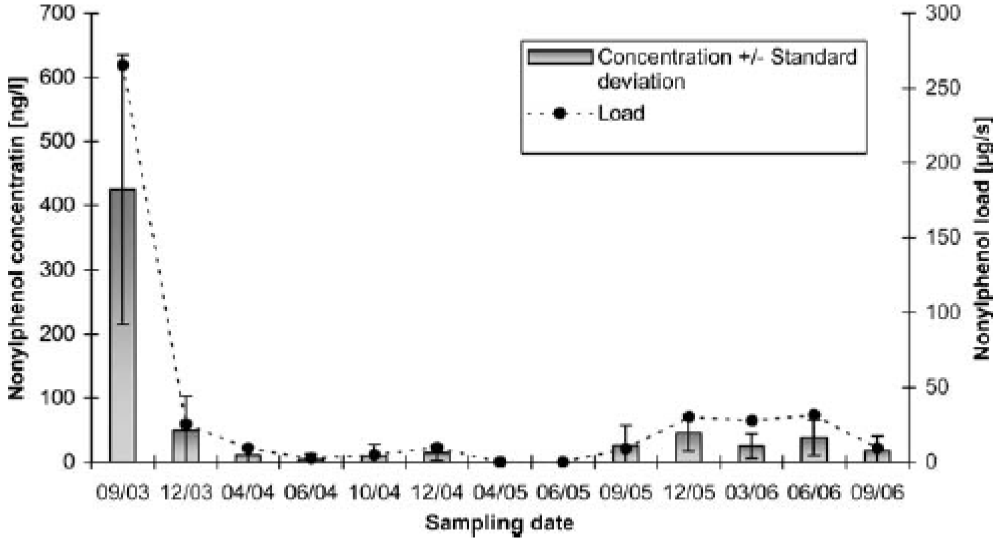

Figure 6: Nonylphenol concentration and load from September 2003 to September 2006 in the rivers of the Hessisches Ried (Quednow and Püttmann 2009)

Alcohol ethoxylates

In 2005, the European replacement of NPE by C10EO3 is expected to result in an added regional C10EO3 concentration for different environmental compartments as given in Table 12. These replacement concentrations come on top of the already existing concentrations of AE as given in Table 11.

Table 12: Regional concentrations resulting from NPE replacement by the AE C10EO3 for different replacement scenarios and different environmental compartments

Compartment	**Regional Surface water**	**Regional Sediment**	**Agricultural soil**
Replacement scenario	µg/L	mg/kg wet weight	mg/kg wet weight
a = 50% AE ww	0.012	0.0004	0.0035
b = 100% AE ww	0.025	0.0008	0.0071
c = 200% AE ww	0.049	0.0016	0.0142

All the exposure estimates resulting from for the BAU and Policy Scenarios for NP and non-replacement AE were literally taken from the appropriate risk assessment documents (EC 2002; HERA 2009 (version 2)), but also largely reproduced by applying the appropriate EUSES calculations. The exposure concentrations for the alternative detergent C10EO3 are derived by applying the EU TGD spreadsheet model, which aims to represent the algorithms described in the 2003-version of the EU Technical Guidance Document, as implemented in EUSES 2.0.3 (EC 2003). The latest version of this model (EUTGDsheet 1.24 (20080418)) was downloaded on 19/7/2001 from the website http://cem-nl.eu/eutgd.html. As input for the model, the continental and regional emissions of C10EO3 for different replacement scenario, as given in Table 10, as well as the physico-chemical properties for C10EO3 were substituted in the model. The relevant properties of C10EO3 are given in Table 13.

Table 13: Physico-chemical properties of NP and our model replacement AE C10EO3 (WCA 2011)

Property	**NP Value**	**C10EO3 Value**	**Unit**
Generic name	Nonylphenol	Alcohol ethoxylate	-
Cas registry number	84852-15-3	68439-46-3	-
Molecular mass	220	290	g.mol^{-1}
Structure code	-	C10EO3	-
Melting point	-2.8	112.71	^{o}C
Vapour pressure	3.29	2.9E-05	Pa at 25 °C
Water solubility	46.08	1.3E+02	mg.L^{-1} at 25 °C
Kow	26915	8913	-
Koc	104712	1462	L.kg-1
Biodegradability	inherently biodegradable	Readily biodegradable	-
Degradation rate in WWTP	2.4	100	d^{-1}
Degradation rate in surface water	4.62E-03	4.16	d^{-1} at 12 °C
Degradation rate in marine water	1.39E-06	4.16	d^{-1} at 12 °C

1.2.3 Step 2c: Hazard characterization

Hazard characterization for BAU and PS

Measured chronic toxicity data for NP in water are given in Table 14. For the calculation of sediment toxicity, the following formula, based on equilibrium partitioning (EP) theory, is applied (EC 2003, Formula 70):

$$Toxicity_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \times Toxicity_{water} \qquad \text{Eq.10}$$

Where:

$Toxicity_{water}$: Observed toxicity in water in µg/L

RHO_{susp}: Bulk density of wet suspended matter = 1150 kg/m^3 as derived from the EU TGD spreadsheet model

$K_{susp-water}$: Water partition coefficient of NP between suspended matter water = 2619 m^3/m^3 as derived from the EU TGD spreadsheet model

$Toxicity_{sed}$: Predicted Toxicity in sediment in mg/kg

Table 14: Chronic freshwater toxicity data for NP (EC 2002) and estimate of sediment toxicity, based on equilibrium partitioning between water and suspended matter

Group	Organism	Endpoint	Criterion	Aquatic toxicity ug/L	Sediment Toxicity mg/kg ww
Crustacea	Ceriodaphnia dubia	7 d NOEC	Reproduction	88.7	202.0
Crustacea	Chironomus tentans	20 d NOEC	Survival	42	95.7
Crustacea	Daphnia magna	21 d NOEC	Surviving offspring	24	54.7
Crustacea	Daphnia magna	21 d NOEC	Reproduction	100	227.7
Mixed	Diverse	30 d NOEC	Endocrine disruption	10	22.8
Plants	Lemna minor	96 h NOEC	Growth rate	125	284.7
Plants	Lemna minor	96 h NOEC	Frond production	901	2051.9
Fish	Lepomis macrochirus	28 d NOEC	Mortality	5.95	13.6
Fish	Mysisdopsis bahia	21 d NOEC	Length	3.9	8.9
Fish	Pimephales promelas	33 d NOEC	Survival	7.4	16.9
Fish	Pimephales promelas	28 d NOEC	Mortality	77.5	176.5
Algae	Scenedesmus subspicatus	72 h EC10	Biomass	3.3	7.5
Algae	Scenedesmus subspicatus	72 h EC10	Growth rate	25.1	57.2
Algae	Scenedesmus subspicatus	72 h EC10	Cell growth	500	1138.7
Algae	Selenastrum capricornutum	96h NOEC	Cell production	694	1580.5

Measured chronic toxicity data for a collection of worst case AE homologues (C13-15 EO7) are given in Table 15. These toxicity data are reported, because no measured toxicity data are available for our model compound C10EO3. To convert aquatic toxicity to sediment toxicity, the same EP formula is applied, with $K_{susp\text{-}water}$ for AE = 37.45 m^3/m^3 as the only difference (also derived from the EU TGD spreadsheet model).

Table 15: Chronic freshwater toxicity data for a range of AE homologues (C13-15 EO7) with worst case characteristics (HERA 2009 (version 2); WCA 2011), **and EP-estimate of sediment toxicity**

Group	Organism	Endpoint	Criterion	Aquatic Toxicity µg/L	Sediment Toxicity mg/kg ww
Algae	Scenedesmus subspicatus	72 h NOEC	Growth	39	1.27
Crustacea	Copepoda Cladocera	30 d NOEC	Reproduction	730	23.77
Fish	Pimephales promelas	28 d NOEC	Growth	1600	52.10

Measured chronic toxicity data for NP as reported in the RAR (EC 2002) are given in Table 16. Where the chronic terrestrial toxicity is only reported as an EC50, the NOEC is extrapolated by dividing by a factor of 3 (Lettuce). EC10 and NOEC are considered equivalent.

Table 16: Chronic soil toxicity data for NP (EC 2002)

Group	Organism	Endpoint	Soil toxicity mg/kg ww
Annelida	Earthworm	21 d EC10 reproduction	3.44
Colembola	Folsomia	21 d EC10 reproduction	27
Plant	Sorghum	21 day NOEC Growth	100
Plant	Sunflower	21 day NOEC Growth	100
Plant	Soya	22 day NOEC Growth	100
Plant	Lettuce	14 day NOEC* Growth	208

For AE, the measured chronic toxicity values for C12EO4 are reported in the HERA RAR (HERA 2009 (version 2)). According to the same document (Table 4.47) the toxicity of C12EO4 is a factor of 3 lower than the toxicity of C10EO3. The toxicity of C10EO3 is extrapolated by dividing the observed toxicity for C12EO4 by 3. Table 17 gives the toxicity of C10EO3 as extrapolated.

Table 17: Chronic soil toxicity data for C10EO3, extrapolated from the measured chronic toxicity data for C12EO4 (HERA 2009 (version 2))

Group	Organism	endpoint	Soil toxicity mg/kg ww
Nematoda	Caenorhabditas elegans	chronic NOEC number of juveniles	73
Colembola	Folsomia candida	chronic NOEC adult mortality	73
Colembola	Folsomia candida	chronic NOEC number of juveniles	73
Nematoda	Caenorhabditas elegans	chronic NOEC adult mortality	153
Annelida	Eisena foetida	chronic NOEC adult mortality	333
Annelida	Eisena foetida	chronic NOEC number of juveniles	333

1.3 Step 3: Determination of endpoints and assessment method

1.3.1 Risk by toxicity driven only

As described by the standard methodology, the method for impact assessment applied depends on the hazard characteristics of the substances used in BAU and PS. The hazards characteristics of both NP/E and AE are based on ecotoxicity only (endocrine disrupting characteristics are in principle assumed to be part of toxicity and are included in the hazard data presented above)[3]. Following the methodology decision scheme for this case study the probabilistic and/or deterministic method can used to estimate the environmental impact of the BUA and PS scenarios. For this case both EIA methods (4b and 4c) will be applied.

1.3.2 Risk characterization for BAU and PS

Before the actual impact assessment will be performed, first the RCRs for all possibly relevant compartments are calculated on the basis of the results from step 2.

Nonylphenol
For the 1997 BAU-scenario, the EU RAR reveals risk quotients for general toxicity as depicted in Table 18 (EC 2002). The risk quotients extrapolated for the 2005 restriction scenario are based on a 70% reduction of the NP emissions (RPA 1999). The risk quotients indicate the highest risk (RCR > 1) for sediment dwelling organisms in the BAU scenario. No risk is shown in the RCR estimations of the Policy Scenario.

Table 18: Risk quotients for the BAU and the 70% restriction scenario for NP, based on general ecotoxicity (EC 2002; RPA 1999)

Compartment	**Scale**	**PNEC**	**PEC**	**Unit**	**PEC/PNEC**	**PEC/PNEC**
Year			**1997**		**1997**	**2005**
Scenario			**BAU**		**BAU**	**70% NP restriction**
Water	Regional	0.33	0.60	µg/L	1.78	0.53
	Continental	0.33	0.07	µg/L	0.22	0.07
Sediment	Regional	0.27	0.10	mg/kg ww	2.64	0.79
	Continental	0.27	0.01	mg/kg ww	0.05	0.01
Soil	Regional	0.27	0.23	mg/kg ww	0.88	0.26
Secondary poisoning Earthworm	Regional	10	0.76	mg/kg ww as food	0.08	0.02
Secondary poisoning Fish	Regional	10	1.69	mg/kg ww as food	0.17	0.05

Concluded from the scarcely reported observations on endocrine disruptive action, the PNEC values for estrogenic activity are estimated to be a factor of 3 higher than the PNEC values reported for general toxicity, thereby reducing the risk by a factor of 3 as compared to Table 11.

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[3] Note that specific tests on endocrine disrupting effects have not been addressed in the standard ecotoxicity tests, so that these may have gone unnoticed in the tests, while they might occur under realistic exposure conditions in the field.

Alcohol ethoxylates

For the 1999 BAU scenario, the combined risk of all 222 likely AE homologues emitted as a consequence of the estimated European use volume of 290,000 tonnes per year (considered to be equal to the European use volume for the year 1997), is presented as the Risk Characterization Ratio (RCR), equal to the sum of the PEC/PNEC values for all the AE homologues. A summary of the RCR values determined for the different environmental compartments is given in Table 19 (HERA 2009 (version 2)).

Table 19: RCR values based on a chronic probabilistic evaluation for total regional AE PECs in the environment (HERA 2009 (version 2))

Environmental Compartment	RCR BAU 1999 = 1997	RCR Worst case Policy Scenario c 2005
Surface water	0.024	0.03
Sediment	0.181	0.23
Soil	0.068	0.09

The RCR values for the BAU scenario are all well below unity, implying a complete absence of environmental risk, and thus a complete absence of impact for the 1999 use of AE detergents in Europe. It seems acceptable to assume that the same holds for the background AE use under the BAU scenario for the year 1997.

The European average emission rate for AE as a consequence of the use of 290,000 tonnes per year is about 800,000 kg/day. Under the Policy Scenario with a 100% ban on the use of NPE, a maximum replacement causing a maximum of extra emission of 216,120 kg/day of AE is foreseen. If we consider the same distribution of AE homologues as adopted for the BAU scenario, this would result in approximately a 25% increase of the RCR values for AE. This still results in risk estimates well below unity.

Relevance of continuation of the impact assessment

Based on this analysis it can be concluded that BAU yields more risk than the Policy Scenario. However, to better estimate the level of improvement of introducing the Policy Scenario, this case will continue the environmental impact assessment analysis. In the impact assessment the environmental compartments surface water, sediment and soil will be included in the assessment, as these show a risk indication of over 0.8. Secondary poisoning is not included as no risk is indicated here.

1.4 Step 4: Environmental impact assessment for BAU and PS

1.4.1 Step 4b: Environmental impact assessment based on a deterministic approach

The actions mentioned in this section refer to the required actions of this impact assessment method as described in section 3.5.2 of the report (environmental impact assessment based on a deterministic approach).

Estimation of European emissions to surface water
For the detergent uses of both NPE and AE, all European emissions are considered to be to fresh surface water after treatment in a properly working WWTP facility.

Prevented emission of NP
According to the RAR (EC 2002) for the use of NPE, this means that 2.5% of the NPE emissions to the European WWTP facilities is emitted to surface water. All considered Policy Scenarios a, b and c (PS) (see section 1.1.2) imply a 100% reduction in the use volume of NPE for the year 2005. This 100% reduction amounts to a prevented NPE emission to waste water of 108,060 kg/day = 3.9E+07 kg/y, equivalent to a prevented NP emission to surface water of 1.0E6 kg/y of NP.

Substitute emission of AE
For the replacement emission of AE with the CAS registry number 68439-46-3 (Alcohols,C9-11 ethoxylated) to waste water, three different scenarios are formulated as depicted in Table 20.

The AE RAR document (HERA 2009 (version 2)) claims a treatment removal exceeding 99% observed in a variety of treatment plants. This results in a 1% emission to European surface waters as presented in Table 20.

Table 20: European emissions of AE to WWTP facilities for different replacement scenarios

Policy replacement scenario	European emission to WWTP facilities kg/d	European emission to WWTP facilities kg/y	1% European emission to surface water in kg.y
a = 50% AE ww	54,030	2.0E+07	2.0E+05
b = 100% AE ww	108,060	3.9E+07	3.9E+05
c = 200% AE ww	216,120	7.9E+07	7.9E+05

Collection of characterization factors
Characterization factors for NP and AE were derived according to the model described the ReCiPe methodology (Goedkoop et al. 2009; Van Zelm et al. 2009). These characterization factors as calculated by Equation 8) are depicted in Table 21.

Table 21: Endpoint characterization factors for ecosystem damage for NP and AE emitted to European freshwaters. Kindly provided by Prof. Dr M.A.J. Huijbregts (Radboud Universiteit, Nijmegen, The Netherlands).

CAS reg. no.	Compound name	$CF_{ED,Freshwater}$ in species.yr/kg
68439-46-3	Alcohols, C9-11, Ethoxylated	6.25435E-10
84852-15-3	4-Nonylphenol, Branched	1.34046E-07

Calculation impact score (IS) BAU and PS and impacts of replacement to species richness in European freshwater systems

This operation is performed by applying Equation 9 (see section 3.5.2 of the report) for two purposes:

- to calculate the increase in the number of species by the reduction in the freshwater emission of NP
- to calculate the decrease of the number of species by the increase in the freshwater emission of AE

Table 22: Impact on biodiversity (number of species) in the BAU and the different Policy Scenarios

Scenario	Impact score NP	Impact score AE	Impact score saldo
BAU	0.14	0.00	-0.14 (0.14 species lost)
PSa = 50% AE ww	0.00	0.00	0.00
PSb = 100% AE ww	0.00	0.00	0.00
PSc = 200% AE ww	0.00	0.00	0.00

1.4.2 Step 4c: Environmental impact assessment based on EUSES exposure modelling and SSDs

Species Sensitivity Distribution (SSD)

Tables 14 and 15, presented in section 1.2.3, can be converted to an aquatic SSD as depicted in Figure 7. The graph for the EP extrapolated SSD for sediments is given in Figure 8. Note that the SSDs are developed on the basis of NOECs instead of EC50s as prescribed by the methodology. Being readily available, using NOECs here can be seen as a lower tier approach. This was found sufficient for this case study to come to conclusive results. An SSD based on NOECs generally differs a half to one order of magnitude from the SSD based on acute HC50 data, the SSD-NOEC being the more sensitive one (see section 3.5.3 of the report). Using HC50 SSDs would thus have resulted in lower impact estimates.

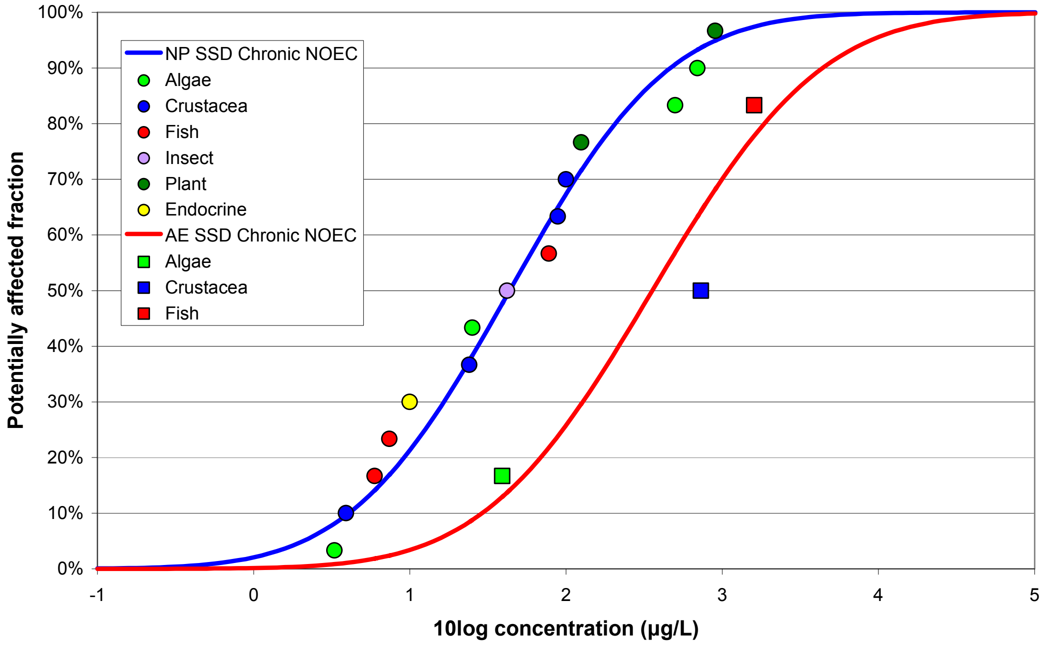

Figure 7: SSD graph for NP and AE in surface water, based on chronic NOEC values for aquatic species

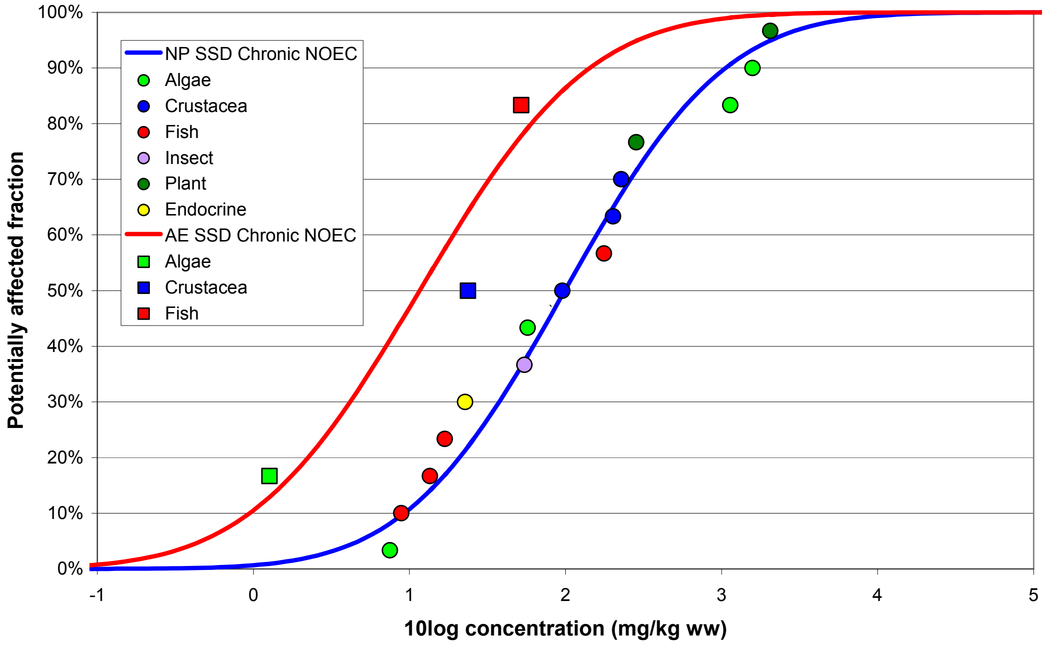

Figure 8: SSD graph for NP and AE in sediments, extrapolated by equilibrium partitioning from chronic NOEC values for aquatic species

In Figure 9, the data from Table 16 and Table 17 are converted to SSD curves.

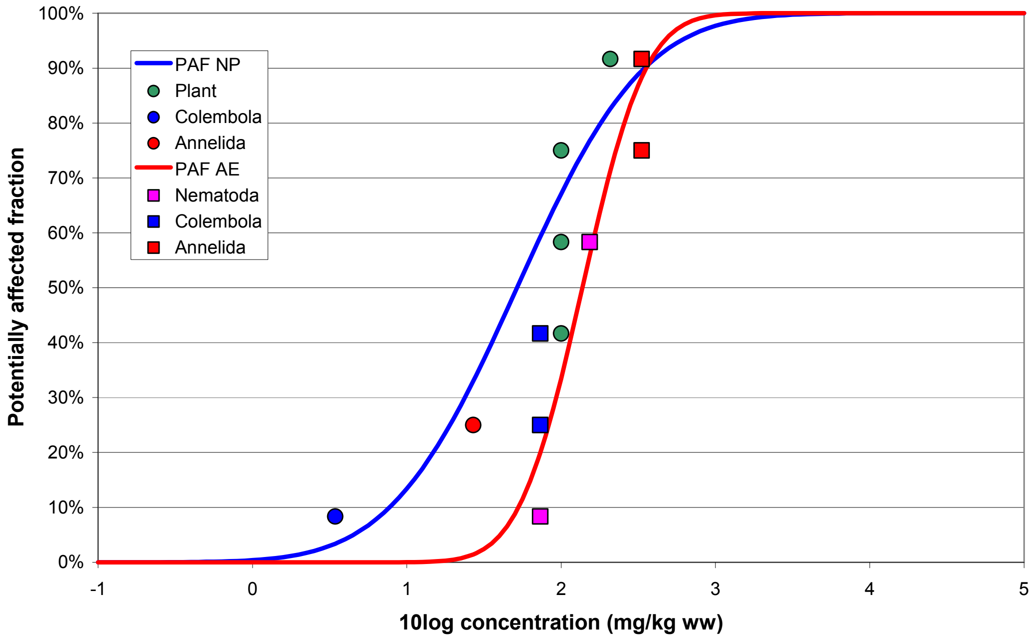

Figure 9: SSD graph for NP and AE C10EO3 in soil

<u>Environmental impact results</u>

For general ecotoxicity, the impact is estimated as the proportion of a generic assembly of species potentially affected by the predicted environmental concentrations of both NP and the AE (C10EO3) replacement for different Policy Scenarios, where the AE replacement concentration is evaluated on top of the 1999 background concentration of a very diverse AE mixture. Because the RCR for the background AE mixture concentration, as calculated by the HERA RAR (HERA 2009 (version 2)), is considerably below unity (Table 23, the impact of the AE background is set to zero).

Table 23: Ecotoxicological impacts as evaluated for the NP to AE scenarios adopted. The impacts are expressed as the Potentially Affected Fraction of a generic species assembly (PAF) for the single compounds NP and AE . For NP and AE together the impact is expressed as the msPAF for a mixture of multiple substances.

SCENARIO				**BAU**	**50% AE ww**	**100% AE ww**	**200% AE ww**
COMPARTMENT	**REGIONAL CONC**	**REGIONAL CONC**	**Unit**	**1997**	**2005**	**2005**	**2005**
SURFACE WATER	**NP**			**PAF NP**	**PAF NP**	**PAF NP**	**PAF NP**
100% NP 1997	0.6		µg/L	1.02%			
30% NP 2005	0.18		µg/L		0.15%	0.15%	0.15%
SEDIMENT	**NP**						
100% NP 1997	0.103		mg/kg ww	0.01%			
30% NP 2005	0.0309		mg/kg ww		0.00%	0.00%	0.00%

SCENARIO				**BAU**	**50% AE ww**	**100% AE ww**	**200% AE ww**
COMPARTMENT	**REGIONAL CONC**	**REGIONAL CONC**	**Unit**	**1997**	**2005**	**2005**	**2005**
AGRI SOIL	**NP**						
100% NP 1997	0.265		mg/kg ww	0.02%			
30% NP 2005	0.0795		mg/kg ww		0.00%	0.00%	0.00%
SURFACE WATER	**Addition C10EO3**	**Background AE-mixed**		**PAF AE**	**PAF AE**	**PAF AE**	**PAF AE**
50% AE ww	0.01225	1.01	µg/L	0.00%	0.00%		
100% AE ww	0.0245	1.01	µg/L	0.00%		0.00%	
200% AE ww	0.049	1.01	µg/L	0.00%			0.00%
		msPAF NP+AE WATER		**1.02%**	**0.15%**	**0.15%**	**0.15%**
SEDIMENT	**Addition C10EO3**	**Background AE-mixed**		**PAF AE**	**PAF AE**	**PAF AE**	**PAF AE**
50% AE ww	0.0004	1.01	mg/kg ww	0.00%	0.00%		
100% AE ww	0.0008	1.01	mg/kg ww	0.00%		0.00%	
200% AE ww	0.0016	1.01	mg/kg ww	0.00%			0.00%
		msPAF NP+AE SEDIMENT		**0.01%**	**0.00%**	**0.00%**	**0.00%**
AGRI SOIL	**Addition C10EO3**	**Background AE-mixed**		**PAF AE**	**PAF AE**	**PAF AE**	**PAF AE**
50% AE ww	0.0035	0.24	mg/kg ww	0.00%	0.00%		
100% AE ww	0.0071	0.24	mg/kg ww	0.00%		0.00%	
200% AE ww	0.0142	0.24	mg/kg ww	0.00%			0.00%
		msPAF NP+AE AGRI SOIL		**0.02%**	**0.00%**	**0.00%**	**0.00%**

1.5 Step 5: Uncertainty analysis

1.5.1 Overview of the uncertainties of this case study

For this case study, different choices and assumptions are made, input data are used and processed and model calculations are performed. All these aspects can cause uncertainty or error to the end results. Table 24 gives an overview of the main sources of uncertainty and error of both the BAU and PS and tries to indicate the possible effects to the end conclusion of the case study.

The only choice with potential implications for the outcome of the risk reduction estimates is the choice for the model replacement AE C10EO3. However, based on a QSAR evaluation (HERA 2009 (version 2)), the intrinsic toxicity of the AE homologues in the range C10EO3 to C14EO10 (most used as detergents) ranges from a factor of 5 less toxic to a factor of 12 more toxic than C10EO3. The PEC of the background AE-mixture concentration in the BAU scenario is considered to yield marginal risk, if any (Table 19). The added replacement PEC leaves a margin of about a factor 90 to 20 for the 50 to 200% Policy Scenarios to equal the background AE concentration (1.1 µg/L background AE (Table 11) versus 0.012 to 0.049 µg/L (Table 12)) of replacement C10EO3. This implies that the choice of AE is immaterial for the outcome of the risk reduction evaluation.

1.5.2 Uncertainties as stated in both RAR documents

The EU NP & NPE RAR (EC 2002)

There are a number of uncertainties in the risk characterization for the aquatic environment, including sediment. Firstly, a number of emission scenarios are based upon default estimations. This may result in significant variations between predicted and actual environmental concentrations.

In the PEC calculations, some of the calculated levels are higher than the water solubility of NP. This could mean that the actual concentrations are overestimated in these cases. The RAR authors decided not to make corrections in these cases.

The results of biodegradations studies show a wide variation in test results. The reasons for this include possible toxicity of NP to the microorganisms in the test system, the level of adaptation of the microorganisms to NP exposure and a varying isomer composition of the NP. Therefore the actual half-life for NP in the environment could be longer or shorter than the estimated values, depending on the prevailing conditions.

In soil and sediments, the measured and calculated values for adsorption coefficients are different. Evidence for measured levels indicates that sorption to particulate material may be governed by factors other than carbon content. The calculated PEC values do not take this into account. The actual adsorption onto soil and sediment may be higher than estimated, thereby reducing the exposure in water.

The PEC calculations assume that NPE is instantly converted to NP in sludge, whereas in the real environment this will be a gradual process. This assumption must lead to conservative PEC estimates in all compartments.

The HERA AE RAR (HERA 2009 (version 2))

The HERA RAR for AE only refers to the uncertainty in the sorption of AE to organic carbon, due to the fact that Koc does not reflect all of the sorption mechanisms for AEs. The RAR claims that the PEC estimates in all compartments are to be considered conservative, based on evidence collected in actual measurements.

Table 24: Overview of sources of uncertainty and error in the end results

Choice/assumption/input data used	Quantitative or qualitative description BAU	Quantitative or qualitative description PS	Validity	Consequence on the result	Data source used and cause of uncertainty
Scope and scenario definition (choices and assumptions)					
(alternative) substance	**NP, NPE and a mix of NPE substances**	**A diverse mixture of AE homologues. This case study assumes C10EO3 as the model replacement. Unclear whether these alternatives cover all restricted applications**	**AEs are the most common replacements for NPE.**	**None, other AE replacements can increase toxicity by a factor 12, this however turns out to be immaterial when it comes to risk or impact evaluation**	**ToxEcology, 2002**
Included applications	Detergent use of NPE	Detergent use of AE	As prescribed by EU legislation	None	2003/53/EC
Replacement ratio alternative	100% of NPE reduction	Replaced by 50-200% of AE (C10EO3)	Variable replacement ratio is applied because of uncertainty in replacement ratio = sensitivity analysis	None, difference in risk and impact between 50-200% replacement ratio is nil/zero	This document
Scope of the impact assessment related to the restriction proposal (production, use, placing on the market)	Scope of impact assessment in line with the restriction: placing on the market and use	-	As prescribed by EU	None	2003/53/EC
Included life cycle stages					
Production stage	Included for NP and NPE	Not included for AE			Both RAR documents
Use stage	Included for NP and NPE	Included for AE	Assumed to be valid	None	Both RAR documents
Waste stage	Included for NP and NPE	Included for AE	Assumed to be valid	None	Both RAR documents

Choice/assumption/input data used	Quantitative or qualitative description BAU	Quantitative or qualitative description PS	Validity	Consequence on the result	Data source used and cause of uncertainty
Import/export	Included for NP and NPE	Not included for AE	Assumed to be valid	None	Both RAR documents
Geographical scale	Europe 15	Europe 15	Only data available for EU 15. New EU countries will, however, also implement the restriction. Is similar for BAU and PS	None	Both RAR documents
Starting point in time of restriction	2005 fully implemented	2005 fully implemented	As prescribed by the EU restriction, and thus valid	None	2003/53/EC
Included time span of use	1997-2005	2005	Valid because of the high turnover rate and high degradability of both compounds	Taking a wider timeframe would not change the conclusions so no consequences on the results assumed	2003/53/EC
Included time span of effect	Days to weeks	Days to weeks	Valid because of the high turnover rate and high degradability of both compounds	Taking a wider timeframe would not change the conclusions so no consequences on the results assumed	Both RAR documents
Assumed trend in use (import, export, production)	No trend assumed, data from years available taken as reference	No trend assumed, quantities assumed based on BAU data and different replacement rates	Assumed to be valid because of short transition time and stagnant population growth/economy	None	Both RAR documents
Choice of relevant ecotoxicity endpoints	General chronic ecotoxicity, endocrine disruption and secondary poisoning	Only general chronic ecotoxicity	No other indicators	None	Both RAR documents

Choice/assumption/input data used	**Quantitative or qualitative description BAU**	**Quantitative or qualitative description PS**	**Validity**	**Consequence on the result**	**Data source used and cause of uncertainty**
Choice of relevant environmental compartments	Surface water, sediment, soil and secondary poisoning	Surface water, sediment and soil. Secondary poisoning not included because not assumed to be relevant	All relevant compartments are included and thus valid. Air is omitted, because both NP/E and AE are hardly airborne	None	Both RAR documents
Input data and model/parameter uncertainties					
Included use amounts	For NP and NPE, the 1997 use amount is included as reference: European use of 78 500 tonnes per year of NP. For AE (background) the 1999 use amount is included as reference: European use of 290,000 tonnes per year	Amounts based on amounts in BAU assuming different replacement ratios	Based on available data	n/a	Both RAR documents
Release estimation					
Air	Included for NP, but not for NPE, since NPE is hardly airborne	Not relevant since AE is hardly airborne	n/a	n/a	Both RAR documents
Water (fresh/sea)	Included for NP and NPE	Included for AE	Releases may be slightly overestimated for both NP and AE due to underestimation of sorption to particulate matter	Hardly any influence, but conservative	Both RAR documents

Choice/assumption/input data used	Quantitative or qualitative description BAU	Quantitative or qualitative description PS	Validity	Consequence on the result	Data source used and cause of uncertainty
Sediment	Included for NP and NPE	Included for AE	Releases may be slightly underestimated for both NP and AE due to underestimation of sorption to particulate matter	Hardly any influence	Both RAR documents
Soil	Included for NP and NPE	Included for AE	Releases may be slightly underestimated for both NP and AE due to underestimation of sorption to particulate matter	Hardly any influence	Both RAR documents
WWTP	Included for NP and NPE	Included for AE	Based on model estimates, assuming that all waste water is connected to WWTP. This might not be the case in all European countries. Higher emissions might therefore occur both in BAU and in PS	If not all waste water is pre-treated in WWTPs, the environmental improvement of the restriction might be underestimated, because the environmental degradation of NP is slower than that of AE	Both RAR documents
Exposure estimation					
Peak load vs. base load	Base load, regional and continental concentrations	Base load, regional and continental concentrations	Due to relatively high degradation rates and relatively low local emissions, locally high concentrations are restricted to minute areas. Local impacts will be fewer in PS than in BAU	Averaged out on larger scale	Both RAR documents

Choice/assumption/input data used	Quantitative or qualitative description BAU	Quantitative or qualitative description PS	Validity	Consequence on the result	Data source used and cause of uncertainty
Combined exposure	NP + background AE	Background AE + replacement AE	As documented	None	This document
Used measurement data	**Available measurement data for Sept 2003 (just after end of BAU period) indicates a concentration range in concordance with the BAU PEC for regional surface water.**	**Available measurement data shows larger decrease of NP concentration in water**	**Valid**	**Shows possible underestimation of environmental improvement of the restriction since possible larger decrease of NP in the environment (-)**	**Quednow and Püttmann 2009**
Hazard assessment					
Included species	In total, 21 toxicity studies available on different taxonomic groups (Table 14 and Table)	In total, 9 toxicity studies available on different taxonomic groups (***Table*** 15 and Table 17)	Limited data available, especially on AE. Increases the uncertainty on hazard, especially for PS	None	Both RAR documents
Knowledge on sensitive species	n/a	n/a	n/a	None expected	Both RAR documents
Specific vs. general impacts	General	General	No other data available	None expected	N/a
Aggregation of impacts	Yes	Yes	None	None expected	n/a
Used assessment factors	None	None	Not needed, results point in the same direction as the RAR. PEC/PNEC results generated with assessment factors	None	Both RAR documents

1.6 Step 6: Comparison of the scenarios

The environmental impact characterization for BAU and PS based on EUSES exposure modelling and SSD (step 4c) indicates a rather low impact of about 1% in terms of the proportion of species affected at the level of ‘species probably lost’ even in the BAU scenario. For the same BAU scenario, the alternative deterministic method (step 4b) predicts the loss of less than a one species per hundred (0.14, which would be equal to a loss of 14 species per 10,000 species). Even for the worst case Policy Scenario of 200% replacement of NPE by AE on a weight-by-weight basis, both evaluation methods indicate that the increased use of AE will not result in any (increased) adverse ecotoxic effects on the level of species disappearing. As calculated with the SSD methodology, the transition from the detergent use of NPE to AE results in an 85% impact reduction only in aquatic species. However, this is 85% of a very small impact. After the transition, the predicted impact is solely attributable to the remaining emissions of NP. From both types of analysis, it is not very well possible to conclude on the taxonomic groups of species that will be affected the most.

It is surprising to see that the BAU scenario is not actually producing a lot of environmental impact in the ecosystem. On the grounds of ecotoxicity alone, the low impact of the use of NPE does not seem to justify the restriction measures taken by the EU. However, the measures taken by the EU may be justifiable in view of human effects and alleged NP properties of endocrine disruption, which were not substantially represented in the case study. Note that as far as the argumentation behind adopting this historical restriction proposal of NP and NPE was tracked, the major reason for the restriction seems to be the potential harm to the environment combined with the assumed low replacement cost to industry and society. Any potential effects on human health are not reported explicitly (COM, 2002)

As has been described in section 1.5 no source of uncertainty was identified that would significantly change the end results of this case study.

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Appendix C: Zinc gutter systems

1.1 Step 1: Scope and scenario definition

1.1.1 *Description of the case*

This case describes a Business As Usual (BAU) scenario of zinc in rain-gutters and the impact on the environment after corrosion and leaching of zinc. It has been shown that leaching of zinc to surface waters resulted in an exceedance of the maximum allowable concentration (Verschoor and Brand 2008). Also, it was found that the measured surface water concentrations indicated that the $PNEC_{add}$, aquatic is exceeded in some, but not all, regional waters in the EU (EC 2010). Sediment PEC_{add} / $PNEC_{add}$ ratios for some, but not all, EU regions point to a potential risk for sediment-dwelling organisms. This conclusion was based on both calculated and measured data.

The alternative Policy Scenario (PS) involves a restriction of production and placing on the market of rain gutters made of zinc. We assume that it is replaced in twenty years by rain gutters made of PVC. Two types of PVC are used: the flexible type that contains a relatively high amount of plasticizers (mainly DEHP), and the rigid type with no plasticizer. Both types of PVC have a small amount of stabilizers (mainly CaZn). So, for the BAU scenario we calculated the exposure and effects of zinc to the environment and for the PS we calculated the exposure and effects of DEHP and zinc from PVC. It is expected that the replacement by PVC reduces the exposure and risk to the environment of substances that leach from rain gutters.

1.1.2 *Background information on zinc and PVC*

Zinc

Zinc is the fourth most common metal in use, trailing only iron, aluminium and copper, with an annual global production of about 12 million tonnes. About 70% of the world's zinc originates from mining, while the remaining 30% comes from recycling secondary zinc.

Worldwide, 95% of the zinc is mined from sulfidic ore deposits, in which sphalerite ZnS is nearly always mixed with the sulfides of copper, lead and iron. There are zinc mines throughout the world, with the main mining areas being China, Australia and Peru. China produced 29% of the global zinc output in 2010.

In the EU, zinc production is approximately 2 million tonnes (Table 25). This is almost similar to the consumption of zinc in the EU. For roofs and gutters approximately 120,000 tonnes are used each year (6%).

Table 25: Production and consumption of zinc metal within the EU (EC 2010)

	1993	1994	1995
Production (tonnes)	2,123,000	2,059,000	2,095,000
Consumption (tonnes) [1)]	1,794,000	1,908,000	2,004,000
Surplus (tonnes)	329,000	151,000	91,000

It is not clear if the total consumption mentioned in this table includes recycled zinc.

This shows that in the EU, from 1993 to 1995, the zinc production is almost equal to the zinc consumption. From this it can be derived that it is rather unlikely that zinc metal will be imported or exported from outside the EU. Also, the production and consumption remains relatively constant over the years.

A total amount of 73 t/y is being released from corrosion of zinc in roofing and gutters to the surface waters in The Netherlands (EC 2010). This is about 29% of the total emission of zinc to surface waters (254 t/y) (EC 2010).

PVC

Polyvinyl chloride (PVC) is synthesised by processing ethylene, from oil or gas, and chlorine from salt, with energy (Figure 10). Its unique properties make PVC the material of choice in many applications, including construction, transportation, electronics and health.

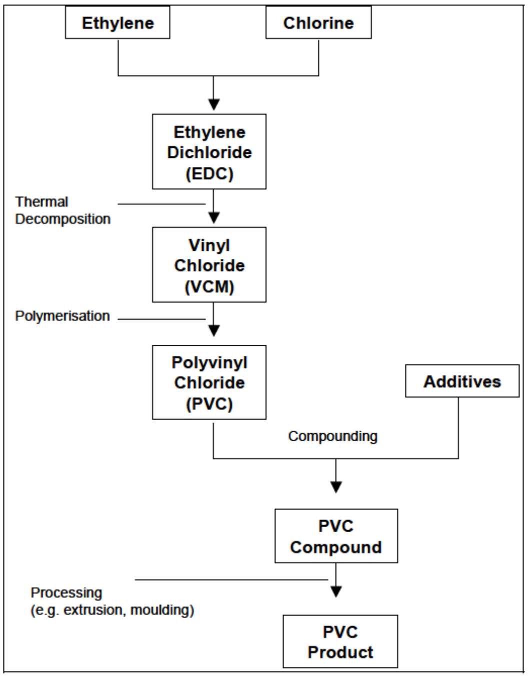

Figure 10: Overview of the PVC product manufacture

PVC is the third most widely used plastic after polyethylene and polypropylene. The European market of PVC resin in 2008 amounted to 6 million tonnes and was growing at around 2% per year. Europe represents about a sixth of the world market. The value of finished PVC products made in Europe is estimated at 75,000 million € and more than 530,000 people are employed by the sector. PVC is efficient in its use of resources, with 57% of its feedstock being salt - one of the earth's most abundant raw materials - and a low energy demand in manufacture. It is also used in many long life applications and can be recycled.

Approximately 30% of the worldwide PVC consumption was used in the EU (5.5 million tonnes) and 2.5% in the Benelux (400,000 tonnes) in 1998 (EC 2004).

Table 26: PVC polymer consumption in the EU by product group in 1999

Use / Application	Percentage	Average life-time (years)
Building	57	10 to 50
Packaging	9	1
Furniture	1	17
Other household appliances[10]	18	11
Electric/Electronic	7	21
Automotive	7	12
Others	1	2 to 10

The building and construction sector is by far the most important PVC sector (Table 26). It comprises almost 50% of applications in relation to the applied mass flow (EC 2004). Window frames, claddings, sheets and conduits/shutter/rails/skirts are all part of this application field, as well as flooring (including sports flooring). Another important PVC application in the building sector is piping. Approximately 12% of applied PVC goes into wastewater and rainwater pipes, and the competitive market share for this application is considered 'major'.

PVC is used in the building sector due to its stability and long life. It requires minimum care and maintenance during the use phase. However, this long lifetime could present a barrier to recycling. Materials deteriorate over time, new technologies are developed, and new restrictions on substances are imposed. With long duration products, old products containing prohibited substances continue to be present in the market. This can pose a problem for the recycling of PVC. Moreover, sometimes it is not possible to identify when the product was produced.

Additives are used to give PVC its specific properties. They are the main concern for toxicological effects. In some cases, additives, such as heavy metals, are being replaced by alternative substances. Cadmium use, for instance, was stopped in 2001, and lead will be phased out by 2015.

Stabilizers

A stabilizer is a complex mixture designed to prevent degradation from heat or UV light. These are added to the PVC polymer to prevent thermal degradation and hydrogen chloride evolution during processing. All PVC is stabilized through the addition of stabilizers.

Plasticizers

Plasticizers are organic compounds, which separate polymer chains, allowing them to move in relation to one other and thereby improve elasticity. The main plasticizer used is DEHP (bis(2-ethylhexyl)phthalate) – see Figure 11 for the production diagram of DEHP.

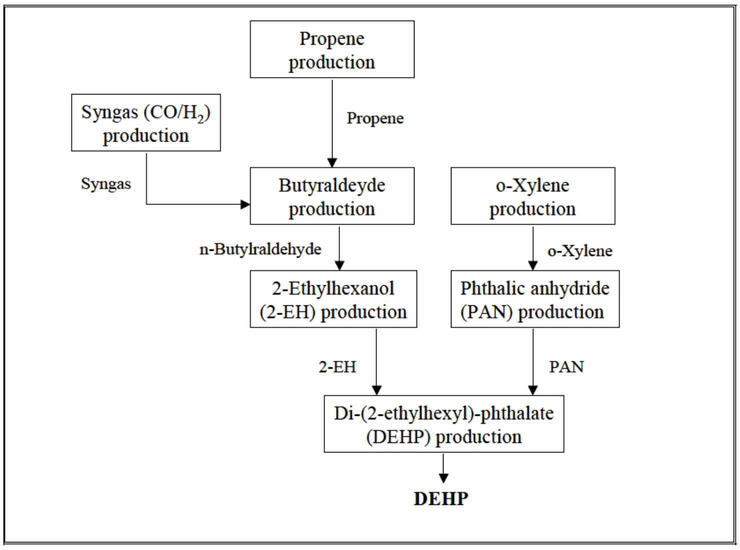

Figure 11: Schematic flow diagram for the production of DEHP

Traces of Phthalates are found everywhere in the environment. They are degraded biologically, especially under aerobic conditions. The contribution of DEHP in rain gutters to these traces is believed to be small.

Fillers
Mainly inert materials such as calcium carbonate (chalk), talc, kaoline, magnesium oxide, etc., which is used to improve some mechanical properties of PVC as well as to reduce costs.

1.1.3 Scenario definition

For the BAU and PS scenario, only the use–lifecycle stage is considered in this case study. Mining, production and waste are not considered, since a recent EU lifecycle analysis has shown that for these stages PVC is considered to be less harmful to the environment (EC 2004). The use stage was not taken into account in the EU study, which makes it opportune to be included in this case study. At a later stage, however, the mining, production and waste stages may be added to the analyses. The geographical scale of the BAU and the PS scenarios is restricted to a typical residential area in the Netherlands of 2000 residents/km^2.

Business As Usual scenario
It is assumed that the amount of gutters made from zinc in the Netherlands remains unchanged during a time period of twenty years. The period of twenty years is used, because this is also approximately the life span of these gutters. A total of 11,000 m^2/km^2 in residential areas is used for the calculations (Table 28). Gutters on new houses that are built during this period are assumed to be made of other material.

Policy Scenario
The Policy Scenario assumes a gradual replacement during twenty years of all gutters made from zinc with gutters made from PVC. New houses that are built

during this period are not taken into account. The replacement is assumed to start in 2011 and ends, when all gutters are replaced, in 2031. It is assumed that in 2011, all gutters are made from zinc and in 2031, all gutters are made from PVC.

Rain gutters made from PVC are assumed to last for approximately fifty years (EC 2004). Two types of PVC gutters are to be used: the rigid type and the flexible type (Table 27). Each is to be used in 50% of the cases. A total of 5500 and 2790 m^2/km^2 is used for the flexible and rigid type respectively (Table 28). Based on the surface area (a measure for the leaching potential), the replacement ratio for zinc:PVC is approximately 1:0.75.

Potential leaching from these PVC gutters is assumed to be low (EC 2004). Only zinc that is used as stabilizer CaZn in most PVC rain gutters and DEHP (diethylhexylphthalate) that is used as plasticizer in flexible PVC are considered in the case study. For the other components in PVC, it was assumed that they did not leach or were not harmful to the environment.

Table 27: Composition of PVC used in the Policy Scenario (in percentage)

Component	**Rigid**	**Flexible**
PVC	92	57
Filler	4	14
Zn as stabilizer (from CaZn)	1.86	1.86
DEHP as plasticizer	0	25
Paraffin (lubricant)	0.7	0.7
Titaniumoxide	0.2	0.2
ABS matrix (25% acrylonitril, 25% butadiene, 50% styrene)	0.1	0.1
Carbon black	0.02	0.02

1.1.4 Choices and assumptions

Table 28: Overview of scenario choices and assumptions

Name	Value (default or assumption)	Remarks (explanation)
Type of housing	Residential area with 2000 residents / km^2	Verschoor & Brand (2008)
Width gutters in the Netherlands	Zinc: 37 cm; PVC: 18 cm for rigid gutters and 37 cm for flexible gutters	Verschoor & Brand (2008)
Area gutters in a residential area	BAU: 11000 m^2/km^2 (37 cm gutters made from zinc) PS: 5500 m^2/km^2 (37 cm gutters made from flexible PVC, used in 50% of the replacements) 2790 m^2/km^2 (18 cm gutters made of rigid PVC, used in 50% of the replacements)	Verschoor & Brand (2008)
Life span	Zinc: 20 years; PVC: 50 years	EC 2004
Leaching rate zinc from zinc gutters	2.51 g/m^2/year	Van Mourik et al. (2003)
Leaching rate DEHP from PVC	0.98 g/m^2/year for the flexible PVC type	See step 2
Leaching rate zinc from PVC	0.008 g/m^2/year for both PVC types	See step 2
Rainwater flow rate	120 m^3/year	Verschoor & Brand (2008)
Background concentration in water	Zinc: 12 ug/L DEHP: 0.33 ug/L	Verschoor & Brand (2008) Struijs & Peijnenburg (2002)

For the Policy Scenario, it is assumed that the zinc gutters are gradually being replaced by PVC gutters during the next twenty years (the expected life span of zinc-gutters). For the PVC gutters, we assume that 50% of the gutters are made of the rigid-type (width of 18 cm – mainly in the Southern part of the Netherlands) and 50% are made of the more flexible type (width of 37 cm – mainly in the Northern part of the Netherlands). The main component that potentially leaches from the rigid PVC type and that may be harmful to the environment is zinc (from the stabilizer CaZn). The main components for the flexible PVC type are the plasticizer DEHP and the stabilizer zinc.

1.2 Step 2: Exposure and hazard assessment

1.2.1 Step 2a: Release estimation

Release estimation for BAU scenario

Leaching rate of zinc from zinc-gutters is set to 2.51 g/m^2/year in The Netherlands (Van Mourik et al. 2003). This rate is derived for residential areas with gutters type ‘Bakgoot 37’, which means that the gutters were 37 cm wide.

Release estimation for Policy Scenario

No measurements or experimental data were found for the leaching rate of DEHP and zinc from PVC. Therefore, these rates were estimated:

Leaching rate of DEHP from flexible PVC

The volume of 1 m^2 gutter (thickness = 1.5 mm) is:

$1000\ \text{mm} * 1000\ \text{mm} * 1.5\ \text{mm} = 1.5 \,.\, 10^6\ \text{mm}^3$

With a density of 1.406 mg/mm^3 (75%) for PVC and 0.985 mg/mm^3 for DEHP (25%) this corresponds to:

$[(0.75 * 1.406)+(0.25 * 0.985)] * 1.5 \,.\, 10^6 = 1.95 \,.\, 10^6\ \text{mg} = 1951\ \text{g gutter}$

If all DEHP would leach from the PVC gutter in the fifty years of the life-span, a weight reduction of 0.5 % · year^{-1} would be appropriate. It was assumed, however, that not all DEHP would leach out during the fifty years. A weight reduction of 0.2 % · year^{-1} was assumed instead.

With a starting concentration of 25 weight% DEHP and a reduction of 0.2 % · year^{-1}, the annual emission rate will be:

$(0.2/100) * (25/100) * 1951 = 0.98\ \text{g/m}^2\text{/year}$

Leaching rate of zinc from rigid and flexible PVC
With a total density of 1.45 mg/mm^3 for PVC, this corresponds to:

$1.45 * 1.5 \,.\, 10^6 = 2175\ \text{g/m}^2\ \text{gutter}$

If all Zn would leach in fifty years, a weight reduction of 0.04 % · year^{-1} would be appropriate. It was assumed that half of the zinc would leach out during the fifty years, which corresponds to a weight reduction of 0.02 % · year^{-1}.

With a starting concentration of 1.86 weight % zinc (Zn) and a reduction of 0.02 weight % · year^{-1}, the annual emission rate will be:

$0.02/100 * 1.86/100 * 2175 = 0.008\ \text{g/m}^2\text{/year}$

1.2.2 *Step 2b: Exposure estimation*

Exposure estimation for BAU scenario
The zinc concentration in the surface water is being expressed as added concentration (C_{add}), due to the present background concentration of approximately 12 ug/L.

The added concentration in the stagnant surface water in a residential area can be expressed as:

$$C_{add} = \frac{A_m \cdot V_m}{A_i \cdot N} \qquad \text{Eq.11}$$

C_{add} = added concentration (ug/L)
A_m = Area of the building material (m^2)
V_m = leaching rate (g/m^2/year)
A_i = rain collecting surface area (approximately 150 m^2 in the residential area)
N = rainfall in the Netherlands (average 0.8 m/year)

The run-off from roofs is being mixed with run-off from streets, which is then being drained away to the surface water. The dilution factor is set to 0.3 (Verschoor and Brand 2008).

The PEC_{added} in surface water was found to be 69 ug/L. Combined with the background concentration of 12 ug/L, this results in a PEC_{total} of 81 ug/L.

Exposure estimation for Policy Scenario

Similarly, PEC_{added} in surface water was calculated for DEHP and zinc in the Policy Scenario. Assuming that 50% of the residents replaced the zinc gutter with flexible PVC and the other 50% replaced it with rigid PVC after twenty years. The PEC_{added} for DEHP would then be 13.4 ug/L in 2031, and for zinc PEC_{added} would be 0.17 ug/L in 2031. Including the background concentration of 12 ug/L for zinc (Verschoor and Brand 2008) and 0.33 ug/L for DEHP (Struijs and Peijnenburg 2002), this results in a total PEC of 12.2 ug/L for zinc and 13.7 ug/L for DEHP. The PEC_{added} for zinc is therefore relatively low compared to the background concentration.

1.2.3 Step 2c: Hazard characterization

Hazard characterization for the BAU and Policy Scenario

EC50 values for aquatic species were collected from the RAR-zinc document (EC 2010) and the RAR-DEHP document (EC 2008) (Table 29). For the calculation of sediment toxicity of DEHP, the following formula, based on equilibrium partitioning (EP) theory, is applied (EC 2008, equation 6 – here 10):

$$Toxicity_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \times Toxicity_{water} \qquad \text{Eq.10}$$

= 3.59 · $Toxicity_{water}$ (mg/kg wwt)
= 9.34 · $Toxicity_{water}$ (mg/kg dwt)

Where:
$Toxicity_{water}$: Observed toxicity in water in μg/L
RHO_{susp}: Bulk density of wet suspended matter = 1150 kg/m^3
$K_{susp-water}$: Water partition coefficient of DEHP between suspended matter water = 4130 m^3/m^3
$Toxicity_{sed}$: Predicted Toxicity in sediment in mg/kg dwt

Table 29: 'Species mean' (geometric average) EC50 values of zinc and DEHP for freshwater organisms, and estimate of sediment toxicity, based on equilibrium partitioning between water and suspended matter

Taxonomic group	EC50 zinc water (ug/L)	EC50 DEHP water (ug/L)	EC50 DEHP sediment (mg/kg dwt)
Algae	143	-	-
Crustacea	80; 225; 305; 465	18,814; 2291	175,723; 21,398
Fish	160; 1300; 1350; 1500; 7800	62,016	579,229
Amphibians	-	22,372	208,954

From these data, a species sensitivity distribution was made (see step 4).

An overall conclusion regarding the toxicity of DEHP to aquatic invertebrates exposed via water in terms of specifying a EC50-value for use in the risk assessment is bound up with problems. There are several indications that the effects observed in the toxicity tests on Daphnia could be caused by physical effects, which probably have no relevance in the environment. There are also indications that DEHP has no shown genuine toxic effect in concentrations up to the water solubility of 3 ug/L (neither the 'true' solubility predicted from the physico-chemical properties nor the 'apparent' solubility found in some toxicity tests). This makes it difficult to interpret the results. For this reason also, no PNEC value in water could be derived for DEHP. There is, however, a PNEC value for sediment of > 100 mg/Kg dw. Using the equilibrium partitioning method, the $PEC_{sediment}$ values were derived from the PEC_{water}.

1.3 Step 3: Determination of endpoints and assessment method

1.3.1 *Risk by toxicity driven only*

As described by the standard methodology, the method for impact assessment applied depends on the hazard characteristics of the substances used in BAU and PS. The hazards characteristics of both zinc and DEHP are based on ecotoxicity only. Following the methodology decision scheme for this case study the probabilistic or deterministic impact assessment methodology is assumed to be sufficient. For this case, the probabilistic impact assessment method will be applied.

1.3.2 *Risk characterization of BAU and PS*

The Maximum allowable Concentration (MAC) for zinc in surface waters is set to 40 ug/L in the Netherlands (Table 30). The Maximum allowable added concentration (MAC_{add}) is set to 28 ug/L and the PNEC-added is 34 ug/L. For DEHP, there are no MAC or PNEC values derived for surface waters due to the problems mentioned earlier.

Table 30: MAC and PNEC values for Zinc and DEHP in water and sediment

	Zinc	**DEHP**	**unit**
MAC total surface water	**40**	Unknown	ug/L
$\mathrm{MAC_{add}}$ total surface water	**28**	Unknown	ug/L
PNEC-added total surface water	34	Unknown	ug/L
PNEC sediment	49	> 100	mg/Kg dw

Risk quotients were calculated for the BAU and PS scenario. PEC/PNEC ratios for the BAU scenario remain 2.0 during the twenty years when only added zinc due to leaching is considered (Table 31). A drop in the ratio is expected for the Policy Scenario to a value below 1. For zinc, the background concentration dominates the risk in this scenario. When only added zinc due to leaching from PVC is considered, a PEC/PNEC in water of 0.006 is to be expected in 2031. For DEHP a PEC/PNEC value below 0.001 is expected in sediments (Table 32).

Table 31: Risk quotients for BAU and PS-zinc in water

	$\mathrm{PNEC_{add}}$ water µg/L	**$\mathrm{PEC_{add}}$ water µg/L**	**$\mathrm{PEC_{add}}$ water µg/L**	**PEC/PNEC**	**PEC/PNEC**
Year		2011	2031	2011	2031
BAU	34	69	69	**2.0**	**2.0**
PS-zinc	34	69	0.2	**2.0**	0.006

Table 32: Risk quotients for PS-DEHP in sediment

	$\mathrm{PNEC_{add}}$ sediment mg/Kg dw	**$\mathrm{PEC_{add}}$ sediment mg/Kg dw**	**$\mathrm{PEC_{add}}$ sediment mg/Kg dw**	**PEC/PNEC**	**PEC/PNEC**
Year		2011	2031	2011	2031
BAU-zinc				**2.0**	**2.0**
PS-DEHP	> 100	0	0.125	0	< 0.001

Relevance of continuation of the impact assessment

On the basis of this analysis, it can be concluded that BAU gives more risk than the Policy Scenario. However, to better estimate the level of improvement of introducing the Policy Scenario, this case will continue the environmental impact assessment analysis.

1.4 Step 4: Environmental impact assessment

A species sensitivity distribution was made from the data in section 1.2 (Figure 12).

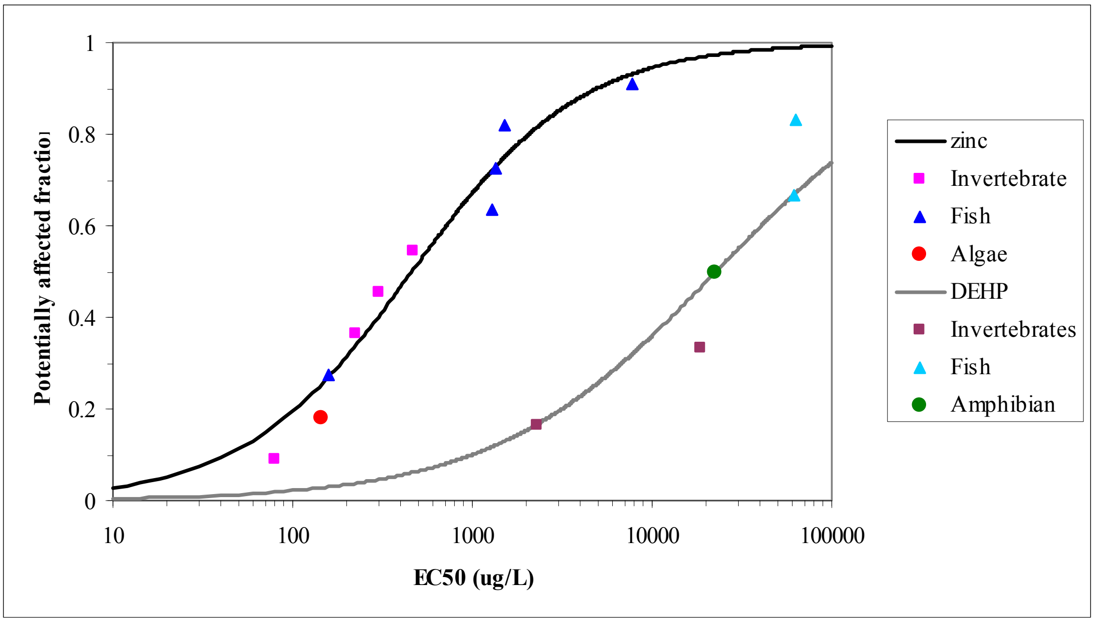

Figure 12: Species sensitivity distributions for zinc and DEHP in water

The SSD curves were used to predict the affected fraction of species from the PEC values which were derived in section 1.2. In the BAU scenario, approximately 15% of the species is affected (mainly mortality), when the zinc concentration due to leaching from gutters is considered (Table 33). When zinc gutters are being replaced by PVC, the affected fraction drops to approximately 0.6% of the species in 2031.

Table 33: Potential Affected Fraction of species (PAF) in the BAU and PS scenario

	BAU **2011-2031**	**PS** **2031**
	PAF zinc	**PAF zinc/DEHP**
Percentage affected species due to zinc/DEHP from gutters	**14.7%**	**0.57%**
Percentage affected species due to total zinc/DEHP (background + from gutters)	**16.7%**	**3.8%**

1.5 Step 5: Uncertainty analysis

The data and analyses shown in this case study contain uncertainty. These uncertainties are addressed in the table below (Table 34). It gives an overview of the main sources of uncertainty and error of both the BAU and the Policy Scenario and tries to indicate the possible effects of this on the end results/conclusion of the case study. Since some of the uncertainties indicate an underestimation of the impact difference between BAU and PS and others indicate an overestimation, no clear conclusion on the overall effect of the uncertainties on the end results can be made.

Table 34: Overview of sources of uncertainty and error in the end results

Choice/assumption/input data used	Quantitative or qualitative description BAU[1]	Quantitative or qualitative description PS[1]	Validity[2]	Consequence on the result[3]	Data source used and cause of uncertainty[4]
Scope and scenario definition (choices and assumptions)					
(alternative) substance	**zinc**	**PVC with zinc and DEHP additives**	**PVC and its additives are widely used as pipes and gutters. It is a realistic alternative substance. However, what additives are/will be used is open for discussion.**	**Dependent on the chosen additives, impact of the PS might differ: +/-**	**Literature and expert judgement**
Included applications	Rain gutters made of zinc	Rain gutters made of flexible and rigid PVC	Both BAU and PS are realistic scenarios	None	Expert judgement
Replacement ratio alternative	Based on surface area - Zinc:PVC = 1:0.75		Rigid gutters are mostly narrower than zinc gutters and flexible PVC gutters	The replaced material in the PS has a lower surface area, which reduces the potential for leaching. It does not underestimate the difference in impact.	Scenario
Included life cycle stages					
Production stage	Not included	Not included	These stages were already studied elsewhere (EC 2004)	None	Not relevant
Formulation stage	Not included	Not included	These stages were already studied elsewhere (EC 2004)	None	Not relevant
Use stage	Zinc in rain gutters	Zinc and DEHP in PVC rain gutters	Emissions in the use-stage were not compared earlier. Therefore, inclusion here is valid.	None	Not relevant
Waste stage	Not included	Not included	These stages were already studied elsewhere (EC 2004)	None	Not relevant
Geographical scale	**Residential area with 2000 residents / km^2**	**Residential area with 2000 residents / km^2**	**These residential areas contain a relatively high gutter density, which may not be representative for other areas in The**	**Overestimation for the rural areas in The Netherlands since the scenario is calculated for**	**Scenario**

Choice/assumption/input data used	Quantitative or qualitative description BAU[1]	Quantitative or qualitative description PS[1]	Validity[2]	Consequence on the result[3]	Data source used and cause of uncertainty[4]
			Netherlands	**residential areas only (+)**	
Starting point in time of restriction	Today	Today	Realistic	None	Scenario
Included time span of use	20 years	20 years	realistic	None	Scenario
Included time span of effect	Days to weeks	Days to weeks	realistic	None	Scenario
Assumed trend in use (production)	none	Increase	realistic	None	Scenario
Choice of relevant eco-tox endpoints	**Only general acute ecotoxicity**	**Only general acute ecotoxicity**	**Valid for BAU, uncertain for PS since fewer data available**	**None for BAU, PS might be over or underestimated. This might thus have an effect on the impact difference between BAU and PS (+/-)**	**Experimental data**
Choice of relevant environmental compartments	Surface water	Surface water, sediment	Valid for BAU. For PS air may be relevant as well	None for BAU. It may be underestimated for PS since secondary poisoning and the air compartment are not taken into account (-)	Measurements
Input data and model/parameter uncertainties					
Included use amounts	11,000 m^2 gutter/km^2	8290 m^2 gutter/km^2	Valid for surface areas.	None	Verschoor & Brand 2008
		1.86% zinc in PVC and 25% DEHP in flexible PVC;	High uncertainty for the composition of the PVC material	May be over- or underestimated	Expert judgement
Release estimation					
Air	Ignored	Ignored	Should be taken into account for PS	Underestimation for PS	Ignored
Water (fresh/sea)	**2.5 g/m^2 gutter/year**	**1 g DEHP/m^2 gutter/year** **0.008 g zinc/m^2 gutter/year**	**valid for BAU, PS is uncertain due to lack of data**	**None for BAU, PS may be over- or underestimated (+/-)**	**Experimental; Lack of data for PS;** Verschoor & Brand 2008
Soil	Ignored	Ignored	valid	None	Ignored

Choice/assumption/input data used	Quantitative or qualitative description BAU[1]	Quantitative or qualitative description PS[1]	Validity[2]	Consequence on the result[3]	Data source used and cause of uncertainty[4]
WWTP	Ignored	Ignored	valid	None	Ignored
Exposure estimation					
Peak load vs base load	Base load	Base load	valid	None	Scenario
Combined exposure	Background zinc+ added zinc	Background zinc+ added zinc + added DEHP	valid	None	Scenario
Specific vs general impacts	general	General	valid	None	Scenario
Used assessment/extrapollation factors	Dilution factor: 0.3	Dilution factor: 0.3	valid	None	Verschoor & Brand 2008
Environmental conditions (temp., rainfall, wind speed, water residence times, etc.)	Rainfall: 800 mm/year Rainwater flow: 120 m^3/year Evaporation/infiltration: 50%	Rainfall: 800 mm/year Rainwater flow: 120 m^3/year Evaporation/infiltration: 50%	valid	None	Verschoor & Brand 2008

1.6 Step 6: Comparison of the scenarios

The BAU and PS scenarios show that the replacement of all zinc gutters in twenty years results in a significant drop in the amount of affected species (around 10-15% of affected species) for the water compartment. This makes PVC gutters the better option in terms of environmental impact caused by chemicals.

Also, when the complete life cycle and other environmental impact categories are considered, the use of PVC (recycled or virgin) is the better option when compared to zinc (environmentally speaking) as is shown in Table 35. The use of recycled materials is, however, preferred over the use of 100% virgin material (EC 2004).

Human health effects, e.g., from DEHP (being the major concern of the substance) are not included in this case study. It is also unclear whether the PVC pipes included in the case study contain DEHP and whether possible human health effects are included in the study. One should thereby recognize that it is a case study performed for methodology testing purposes.

The uncertainty analyses indicated sources of uncertainty that might have an influence on the end results. At first, the additives used in PVC gutters are uncertain. Although zinc and DEHP are plausible additives, other additives might also be used. The geographical scale was restricted to a residential area with a relatively high gutter density, resulting in an overall overestimation of exposure and thus impacts. In the choice of relevant environmental endpoints, only general acute ecotoxicity was included. Further attention to specific mechanisms of action (e.g., endocrine disruption) and chronic studies especially for DEHP might influence the end results. The release estimation for PS is fully based on assumptions resulting in a possible over- or underestimation of the environmental concentration of PS. The overall effect of these major sources of uncertainty can affect the results in two directions.

Table 35: Summary of the analysed impacts during the life cycle of pipes made from zinc and PVC (EC, 2004)

	Zinc pipe (100%)	**PVC pipe (100%)**	**Zinc (40% recycled)**	**PVC (9.3% recycled)**
Overall life cycle	For impacts in terms of consumption of natural resources and potential impacts (such as greenhouse effect and acidification) zinc ranges from 1.6 to almost 5 times more than PVC pipes (100%) in various categories. The largest differences are in air and water pollution (almost 5 times that of PVC).		There is less of a discrepancy between the impacts of recycled zinc and recycled PVC. Values for zinc range from 1.24 to almost 3.5 times the impacts of recycled PVC. The major differences are in the areas of water pollution (3.5x) and air pollution (3x).	
	Zinc consumes less water (0.8 m^3) than PVC (1.9 m^3).		Zinc consumes less water (0.5 m^3) than PVC (1.7 m^3). The consumption of cooling water is much larger for plastic production than metallurgy.	
	Zinc (100%) creates 357 kg of landfill waste in comparison to 2.6 kg by PVC (100%). This is mainly due to zinc extraction in the mine.		Recycled zinc pipes create 214 kg of landfill waste compared to 2.5 kg by recycled PVC. Recycling is considered the environmentally favourable option for both PVC and zinc.	

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Appendix D: HBCDD in EPS

1.1 Step 1: Scope and scenario definition

1.1.1 Description of the case

This case study concerns the restriction of HBCDD in expanded polystyrene (EPS) and the replacement of Hexabromocyclododecane (HBCDD) by another brominated flame retardant Dibromoethyldibromo-cyclohexane (TBECH). For methodology testing purposes, an additional alternative tris (2-chloroethyl) phosphate (TCEP) is considered for the PBT assessment only.

Hexabromocyclododecane (HBCDD)
This case study concerns the substance Hexabromocyclododecane (HBCDD) with CAS registry numbers 25637-99-4 and 3194-55-6 (1,2,5,6,9,10-HBCDD). The focus in this case study is therefore similar to the main focus of the EU risk assessment report (EC, 2008). The EC risk assessment report mentions that there are no differences in molecular structure or properties between the chemicals represented by these CAS registry numbers. Because the latter chemical is the most specific due to the included numbering, the calculations for the PBT assessments correspond to HBCDD with CAS registry no. 3194-55-6. HBCDD is a brominated flame retardant consisting of twelve carbon, eighteen hydrogen and six bromine atoms all tied to the carbon ring, as seen in Figure 13. Its main application is in extruded (XPS) and expanded (EPS) polystyrene foam, mostly used as thermal insulation for buildings. XPS and EPS together cover about 96% of the total HBCDD use in Europe. The remaining HBCDD is used in High Impact Polystyrene (HIPS) and textiles.

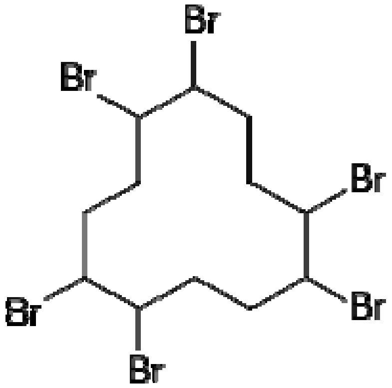

Figure 13: Structural formula of HBCDD

HBCDD is hazardous for the environment and human health. For the environment, the substance is classified with N; R50/53 as agreed at a Technical Committee meeting for Classification & Labelling (TC C&L) on 11-12 June, 2003. This means that the substance is toxic and non-readily degradable. In 2011, the substance is placed on Annex XIV (Authorisation) of REACH Regulation (EC) No. 1907/2006, because the substance meets the criteria of Article 57(d) of a PBT substance. For health effects, the Swedish Chemicals Agency proposed for harmonised classification and labelling HBCDD to be classified as Repr Cat 3; R62 (possible risk of impaired fertility), R63 (possible risk of harm to the unborn child) and R64 (may cause harm to breastfed babies) (CHL report, 2009). In Table 36 below, basic physical and chemical properties are presented that are essential input parameters for the calculation of the environmental concentrations as presented further on in this case study.

Table 36: Basic Physical and Chemical properties of HCBDD (EC, 2008 and Epi Suite)

Name	**Value (default or assumption)**	**Unit (explanation)**
Hexabromocyclododecane, CAS Registry No.: 3194-55-6, EINECS No.: 221-695-9		
Physical and chemical properties		
Molecular weight	641.7	$g.mol^{-1}$
Melting point	190	°C
Vapour pressure at the temperature of the data set	1.6E-05	Pa
Temperature at which vapour pressure was measured	20	°C
Water solubility at the temperature of the data set	6.6E-02	$mg.L^{-1}$
Temperature at which solubility was measured	20	°C
Log Kow (Octanol-water partition coefficient)	5.62	QSAR (EPIWIN)

Alternatives of HBCDD

Dibromoethyldibromo-cyclohexane (TBECH)
According to the European Chemicals Agency (ECHA), there are currently no commercially or technically viable alternatives for HBCDD as a flame retardant in polystyrene foam, as all alternative flame retardants noted impairment of the structure and properties of the EPS foam, making it unsuitable for use in this application (ECHA, 2009a).

In contrast to this document, according to the HBCDD Risk Management Evaluation within the frame of the POP Stockholm Convention there are technically and commercially feasible alternatives available to the different materials in which HBCDD is used on the market, although there are differences in the production process (RME draft, 2011). Alternatives of HBCDD include flame retardant substitution, resin/material substitution and product redesign. Several of these alternatives are considered to be possible suitable candidates (ECHA 2009a, SWEREA 2010, KLIF 2010). However, they may present other risks that need to be taken into account prior to take final decisions.

Some commercially available brominated flame retardants may, however, be used in EPS foam, such as, tetrabromo-cyclooctane, dibromoethyldibromo-cyclohexane (LSCP, 2006) and TBBPA, but a detailed analysis of their effectiveness in this application when compared with HBCDD is not available (Morose, 2006). For the current exercise the impact assessment considers replacing HBCDD within EPS with dibromoethyldibromo-cyclohexane (TBECH) (CAS registry no. 3322-93-8). For TBECH, information – although limited – appeared to be accessible and available. The physical and chemical properties of the substance TBECH essential for the environmental impact calculation are presented in Table 37 below. Dibromoethyldibromo-cyclohexane has not been classified according to Directive 67/548/EEC (http://esis.jrc.ec.europa.eu/index.php?PGM=cla). The substance is, however, found in beluga whales in the Arctic; modelling studies identified that it was likely to be persistent and bioaccumulative; and it was also found to be a strong androgen agonist and mutagenic to mammalian cells *in-vitro* (Draft RME, 2011).

Table 37: Physical and Chemical properties of dibromoethyldibromo-cyclohexane (EPI Suite; Nyholm, 2009; HSDB, 2011)

Substance Property	Value	Unit
Dibromoethyldibromo-cyclohexane (TBECH), CASreg. no.: 332-293-8, EINECS-No.: 222-036-8		
Physical and chemical properties		
Molecular weight	427.8	$g.mol^{-1}$
Melting point	73	^{o}C
Vapour pressure at the temperature of the data set	1.4E-02	Pa
Temperature at which vapour pressure was measured	20	^{o}C
Water solubility at the temperature of the data set	6.9E-02	$mg.L^{-1}$
Temperature at which solubility was measured	20	^{o}C
Log Kow (Octanol-water partition coefficient)	5.24	QSAR (EPIWIN)

Tris (2-chloroethyl) phosphate

According to the EU risk assessment report, historically the largest field of application of TCEP (80-90% of the quantity produced) was the reduction of the brittleness while maintaining the flame-resistant finishing of the polyurethane in the production of celled, rigid or semi-rigid foam. The addition of 10% TCEP relative to the finished foam is sufficient to achieve a clear flame retardant effect. Currently, TCEP is mainly used in the production of unsaturated polyester resins used in the building industry (roof insulation). Other fields of application are acrylic resins, adhesives and coatings.

Knowing that TCEP is technically not a suitable alternative for HBCDD, it is included as an alternative in this study because of its different physical and chemical properties (Table 38) and environmental behaviour compared to two brominated flame retardants HBCDD and TBECH. TCEP is used to specifically test the PBT assessment part of the methodology.

Table 38: Physical and Chemical properties of tris (2-chloroethyl) phosphate (EC, 2009c)

Substance Property	Value	Remark
Tris (2-chloroethyl) phosphate (TCEP), CAS reg.no.: 115-96-8, EINECS-No.: 204-118-5		
Physical and chemical properties		
Molecular weight	285.49 g/mol	EC (2009c)
Melting point	< -70 °C	EC (2009c)
Vapour pressure	0.00114 Pa 20 °C	EC (2009c)
Water solubility	7820 mg/L at20 °C	EC (2009c)
Octanol-water partition coefficient log Kow	1.44	QSAR (EPIWIN)
Organic carbon partition coefficient	Koc 110.2	Estimated, EC (2009c)

1.1.2 *Scenario definition*

As mentioned earlier, this case study assesses the (ecotoxicological) environmental impact of a restriction on HBCDD as a flame retardant in EPS assuming that HBCDD is replaced for this use by TBECH or TCEP. The case study includes two main scenarios for which the environmental impact will be determined and compared: the Business As Usual (BAU) - in which HBCDD is continuously used - and the Policy Scenario (PS) - in which HBCDD is banned and replaced by an alternative flame retardant. The PS is divided into three variants as described in the section below.

For all scenarios, Europe is selected as the geographical scale both in terms of use and in terms of impacts. The service life time of EPS used in insulation material in buildings varies considerably from thirty up to a hundred years with an average of fifty years (ECHA, 2009a). The latter document describes releases from all life cycle steps and specifies release data for all life-cycle steps, except the waste stage. In this exercise, scenarios are compared assuming no specific transition period. The corresponding impact assessments should therefore be compared as independent situations without any influence from the BAU scenario. This means that in the case EPS is produced with the alternative, it is assumed that no stocks with HBCDD are existing and therefore do not need to be treated/replaced either. As replacement of a substance is always a step-wise process, it should be said that this assumption is not realistic. However, it is sufficient for the present cases.
On the basis of the information presented in the previous section, we assume toxicity and PBT characteristics to be the relevant environmental endpoints for both HBCDD and TBECH. The aquatic environment and secondary poisoning are the environmental endpoints focused on in this case study. Since EPS is widely used and production is not limited to very few sites or countries (n>1), the focus of this case study is on regional impacts.

<u>Business As Usual scenario</u>
In the impact assessment of this case study, the emission rates of the year 2006 (Table 39) are taken as a reference. In the BAU, it is assumed that HBCDD will not be restricted and production and use volumes of HBCDD will remain the same as in the year 2006. As can be seen in Table 39, HBCDD use has increased over the last years. Consequently, one may also expect increased emission rates, if no additional risk management measures are adopted. Note that the placing of HBCDD on Annex XIV of REACH (Authorisation) is not included in this Business As Usual Scenario.

Table 39: Use of HBCDD in EPS in the EU (tonnes) (ECHA, 2009a).

Year	EPS
2002	3452
2003	4053
2004	4270
2005	4690
2006	5301
2007	5652

ECHA estimated the total use of HBCDD about 11 tonnes/year in 2006 (ECHA, 2009a). Since 5.3 tonnes were used for EPS in 2006 this equals about 45% of the total HBCDD use. Leaching of HBCDD out of EPS is considered to be the main source of environmental pollution. In practice, this will mainly occur during service-life and possibly during the waste stage. For this exercise, the PECs for surface water and secondary poisoning have been calculated.

Policy Scenario

For the Policy Scenario (PS), it is assumed that the production, placing on the market and use of HBCDD containing EPS is restricted in the European Union from 2007 onwards. In this case, it is assumed that the use will also include export.

PS1. Replacement of HBCDD by TBECH in EPS: In this scenario it is assumed that the substance TBECH is used as alternative of HBCDD within the EPS product. It is assumed that the replacement of HBCDD will take place at once after entry into force of the restriction; so no transition period will be applied. Like HBCDD, also TBECH is a brominated flame retardant. For this exercise, it is assumed that TBECH has the same fire resistance as HBCDD. As TBECH has the same bromine content as HBCDD it is assumed that the same use quantities as for HBCDD can be used (replacement ratio of 1:1 based on weight). Release fractions of TBECH for industrial use and service life are different (higher) compared to HBCDD. Release fractions for TBECH are based on OECD (2009). Similar to HBCDD, leaching of TBECH out of EPS is considered as the main source of environmental pollution. Similar to HBCDD, PECs for surface water and secondary poisoning will be calculated. Soil/sediment is not considered.

As described in section 1.1.1, the sub-section on alternatives, there is not one main alternative for HBCDD in EPS. For this case study, we chose TBECH as the alternative mainly because of its assumed technical and economic feasibility in the EPS application and because of the (although still poor) data availability. In addition, two alternative Policy Scenarios have been included, i.e., PS2 and PS3.

PS2. Replacement of HBCDD in EPS by another non-brominated flame retardant substance, TCEP: This alternative scenario is included to be able to test the ranking methodology presented later on in this study a bit more extensively. Similar assumptions as in PS1 are made in terms of use quantities and fire resistance.

PS3. Replacement of HBCDD containing EPS by an alternative (non-EPS) isolation material: In this case, not only HBCDD needs to be included in the environmental impact assessment, but also the EPS material itself (BAU) and the alternative material (PS) replacing EPS not containing flame retardant chemicals. In this case, other than ecotoxicity environmental impact categories might become relevant also. Similar assumptions as in PS1 and PS2 are made in terms of use quantities and fire resistance. In this case study, this scenario is not fully worked out as the scope of the BAU scenario does not include the EPS material itself and the methodology only allows including ecotoxicity as environmental endpoint at this moment. The scenario, however, was included to show that fundamentally different alternatives might also be possible and relevant.

1.2 Step 2: Exposure and hazard estimation

1.2.1 Step 2a: Release estimation

Release estimation for BAU and PS scenario

For the BAU scenario the releases of HBCDD from EPS in all life-cycle stages (ECHA, 2009a) are summed for the year 2006. For the calculation, the total release during the entire life-cycle, the sum of regional and continental releases is considered. In this case study, it is assumed that all emissions occur in the year the EPS is 'put into operation' (= first year of use/placing on the market). The gradual release that will probably occur in practice is thus not accounted for.

Table 40: Release of HBCDD during each life-cycle stage in 2006 (ECHA, 2009a).

Life-cycle stage	Compartment	Total (kg) (in 2006)	Regional	Continental
Formulation	Air	24,3*	0,5	23,8
	Wastewater	60*	0,0	60,0
	Surface water	264*	141,6	123,2
Industrial use	Air	159	15,9	143,1
	Wastewater	128	12,8	115,2
	Surface water	31	3,1	27,9
Professional and private use	Air	220	22,0	197,8
	Surface water	220	22,0	197,8
Service life	EPS	12,5	1,2	11,2

* The reported releases were total releases for EPS and HIPS formulation and were corrected by 0,8 (80% EPS and 20% HIPS).

Both regional and continental release fractions to various environmental compartments are calculated by dividing the sum of the total releases by the compartment specific release. No division is made for regional or continental emissions.

Table 41: Releases from use of HBCDD and TBECH (kg/year) for the different scenario's considered (based on HBCDD releases in 2006).

Scenario	Release	Total (kg)	Regional emissions	Continental emissions	Regional emissions (kg/day)	Continental emissions (kg/day)
For BAU	Releases (kg/year) of HBCDD from uses in the EU27 in 2006					
	Air	649	82	568	0,225	1,56
	Wastewater	1553	669	884	1,83	2,42
	Surface water	924	361	563	0,99	1,54
For PS1	Releases (kg/year) of HBCDD from use in EPS in 2006					
	Air	416	40	376	0,109	
	Wastewater	188	12,8	175,2	0,04	
	Surface water	515	167	349	0,46	
For PS1 and PS3	Releases (kg/year) of HBCDD from uses in the EU27 in 2006. excl. use in EPS					
	Air	234	42	192	0,116	0,53
	Wastewater	1365	656	709	1,80	1,94
	Surface water	408	194	214	0,53	0,59
For PS3	Releases (kg/year) of TBECH from uses in EPS in 2006					
	Air	1706	170,6	1535	0,5	4,2
	Wastewater	267	26,7	240	0,1	0,7
	Surface water	731	73,1	658	0,2	1,8

The data presented above all relate to the release of HBCDD and TBECH and are needed to calculate the Predicted Environmental Concentration (PEC) and the Potential Affected Fraction (PAF) of the BAU, PS1 and PS3. PS2 is not included as TCEP was only included to test the PBT ranking method and no release and exposure estimate is required for this method.

1.2.2 *Step 2b: Exposure estimation*

Exposure estimation for BAU and PS scenario

The release fractions as presented in Table 8 above are inserted into the spreadsheet version of EUSES, together with the total emission and physical and chemical properties of both HBCDD and TBECH, in order to calculate the potential exposure via surface water of HBCDD and TBECH in terms of predicted environmental concentrations ($PEC_{surfacewater}$, regional). These exposure estimations are presented in Table 48.

1.2.3 *Step 2c: Hazard characterization*

Hazard characterization for BAU and PS scenario

For the estimation of the potentially affected fraction of species (PAF), the Species Sensitivity Distribution (SSD) of the substance has to be known for a specific environmental compartment. The SSD can be determined from measured laboratory toxicity data for different species. For the substances considered in this case study (HBCDD and TBECH), the number of data is too limited to determine the SSD for the aquatic compartment. Therefore, in order to perform the calculation of the PAF, a QSAR model has been used in order to generate additional toxicity data. The ECOSAR model has been applied to this purpose. In deriving the SSD only chronic toxicity, data from the ECOSAR model have been used next to measured chronic toxicity data. The chronic data for aquatic species for both HBCDD and TBECH are presented in Table 42.

Table 42: Overview of chronic toxicity data for aquatic species for the determination of the species sensitivity distribution function (SSD)
Note 1: calc. values calculated by ECOSAR model (US-EPA, 2004) ; meas. Values based on measured toxicity data
Note 2,3,4: data taken from EC (2008)
Note 5: Nyholm (2009)

The ECOSAR model uses the log K_{ow} to estimate the toxicity of the substances, and the underlying assumption is that the toxic mode of the substance is caused by polar narcosis. The typical value of the standard deviation for substances acting through polar narcosis is 0.7, which holds for both substances. The average value of the toxicity data is determined by the value of the log Kow, which for both substances is nearly the same, resulting in comparable values, although HBCDD being slightly more toxic.

1.3 Step 3: Determination of endpoints and assessment method

1.3.1 Risk driven by persistent, bioaccumulative and toxic properties

In this chapter the endpoints and impact assessment method for this case study are chosen. The decision scheme as presented in Figure 2 (overview of the methodology) tells us that if the risk of one of the substances (BAU and PS) is not driven by toxicity only; besides the standard impact assessment based on SSD methodology (probabilistic or deterministic) a ranking method needs to be applied as well to deal with PBT and (if relevant) LRT characteristics. As described in section 1.1.1, HBCDD is classified as toxic to the environment and is also found to comply with the PBT criteria. For TBECH very little is known about its hazardous characteristics, however, it is thought to be persistent and bioaccumulating. For both BAU and PS (1,2 and 3), the PAF and ranking methodology are applied to come to an estimation of the tox-based environmental impact assessment.

1.3.2 Risk characterization of BAU and PS

RCRs of the water compartment
To estimate whether it is useful to do an impact assessment based on a SSD method (step 4b or c) besides the PBT ranking, RCRs are calculated for the different scenarios.
In order to calculate the risk characterization ratio's (RCR), the PEC needs to be divided by the PNEC for the various scenarios.

The PECs that are used, are calculated using EUSES and represent regional concentrations. The physical and chemical properties and emission data used as input in EUSES are presented in Tables 36 and 37 (physical and chemical properties of HBCDD and TBECH) and 41 (release data of HBCDD and TBECH). The following PECs are used:

BAU
$PEC_{HBCDD\ all\ applications\text{-}EPS}$ = 2.1 10^{-6} µg/L
$PEC_{HBCDD,\ EPS}$ = 1,1.10^{-6} µg/L

PS1
$PEC_{\text{HBCDD all applications-EPS}} = 2.1\ 10^{-6}$ µg/L
$PEC_{\text{TBECH, EPS}} = 1.4\ 10^{-7}$ µg/L

PS3
$PEC_{\text{HBCDD all applications-EPS}} = 2.1\ 10^{-6}$ µg/L

For the BAU scenario, RCR belonging to HBCDD all applications-EPS and the RCR belonging to the PEC HBCDD, EPS should be added.

For PS1, the RCR belonging to HBCDD all applications-EPS and the RCR belonging to the PEC TBECH, EPS should be added.

For PS3, the RCR belonging to HBCDD all applications-EPS should be calculated.

The PNEC concentrations are not scenario but substance based. The following PNECs are used:
HBCDD = 0.31 µg/L (EC, 2008)
TBECH = 4 µg/L (Lowest NOEC/10 (40 µg/L /10), Nitocra spinipes from Nyholm, 2009)

For the various scenarios, the following RCRs have been calculated:

$RCR_{BAU} = 2.1\ 10^{-6} / 0.31 + 1.1.10^{-6} / 0.31$ µg/L = $1.03.10^{-5}$ µg/L
$RCR_{PS1} = 2.1\ 10^{-6} / 0{,}31 + 1.4\ 10^{-7} / 4 = 6.8.10^{-6}$ µg/L
$RCR_{PS3} = 2.1\ 10^{-6} / 0.31 = 6.77\ 10^{-6}$ µg/L

As can been deduced from these numbers, the RCRs of PS1 and PS2 do not differ from each other. In general, all scenarios are far below 1.

RCRs of secondary poisoning
In order to calculate the risk of secondary poisoning the PEC/PNEC ratio is calculated as following:

$$PEC = 0.5 * (PEC_{localfreshwater} + PEC_{regionalfreshwater}) * BCF_{fish} * BMF_1 \quad \text{Eq.11}$$

According to the EC (2008) for HBCDD, the PEClocal for freshwater = 1.2 µg/L (annual average). This number represents the formulation of HBCDD for EPS and HIPS and was therefore multiplied by 0.8 (see explanation Table 5) to get the PEC for the formulation of HBCDD for solely EPS (=0.96 µg/l (annual average)). The PECregional for freshwater is reported to be 0.028 µg/l (annual average) (Site J). The BMF for the three diasteriomers of HBCDD range from 4.2-9.2. In the risk assessment report, a BMF of 10 is used for the calculation of secondary poisoning. Using these numbers within Eq. 11 the PEC equals 111 $mg.kg_{wwt}^{-1}$.

According to the EC (2008) for HBCDD, the PNEC for secondary poisoning equals 5 $mg.kg_{wwt}^{-1}$. Dividing PEC by PNEC the risk ratio for secondary poisoning equals to 22.2.

The BMF for TBECH and TCEP are default values based on the log Kow or the BCF for fish as described in the TGD (EC, 2003) and Lijzen et al. (2004). For

TBECH and TCEP with a log K_{ow} of respectively 5.24 and 1.78 and a log BCF of 3.3 and 0.7 the BMF value is 2 and 1 for TBECH and TCEP respectively. For TBECH, however, no suitable PNEC value was found, and therefore no PEC/PNEC ratio was calculated.

The highest PEClocal for TCEP is 37.1 µg/L and the PECregional is 0.09 µg/L. This results in PEC for secondary poisoning of 0.1 mg/kgwwt-1.
The PNECoral for TCEP has been derived from the most critical NOAEL of 44 mg/kgbw/d for rats (EAA, 2009). Applying a conversion factor of 20 for adult rats and an assessment factor of 30 for chronic NOAEL to NOEC the PNECoral is 29.3 mg/kgwwt. The resulting risk ratio for secondary poisoning is approximately zero and therefore negligible.

Table 43: Input values for the calculation of RCRs secondary poisoning HBCDD, TBECH and TCEP

	HBCDD (BAU)	TBECH (PS1)	TCEP (PS2)
PEClocal	0.96 µg/L	n.a.	37.1 µg/L
PECregional	0.028 µg/L	n.a.	0.09 µg/L
BCFfish	19673	18200	11
BMF fish-fish/fish-bird	4.2-9.2; 10	2	1
PECsec poisoning	111 mg.kg_{wwt}^{-1}	n.a.	0.1 mg.kg_{wwt}^{-1}
PNECmammals (rat)	5 mg.kg_{wwt}^{-1}	n.a.	29.3 mg.kg_{wwt}^{-1}
RCRmammals	22.2	n.a.	≈ 0

Overview
Except for secondary poisoning of HBCDD, all RCRs presented above are well below 1, and according to the regular interpretation of RCRs no risk and thus no impact is expected. Following the methodology, only PBT ranking needs to be performed for this case study. However, as the case studies are performed to test the methodology, impact assessment based on step 4b including point source exposure estimates is performed for this case study.

1.4 Step 4: Environmental impact assessment

1.4.1 Step 4a: PBT ranking

As defined in step 3 in the previous section, for this case study a PBT assessment needs to be performed next to the environmental impact assessment. For HBCDD, TBECH and TCEP, the PBT assessment has been performed in order to get an indication of the persistent, bioaccumulation and toxic characteristics of the different substances and to be able to compare these for the various substances. The section below the P, B and T scores for HBCDD, TBECH and TCEP are presented. For equations used to calculate the scores are presented in section 3.5.1 of the methodology chapter of the report. The overall methodology and generation of input data to calculate the P and B scores using QSARs (EPIWIN) is described in detail by Rorije et al. (2011).

P scores
The P scores are calculated using Equation 1. The results are presented in Table 44.

Table 44: Pov and P scores for HBCDD, TBECH and TCEP. The Pov values are based on values calculated by EPIWIN.

Substance	Pov (days)	P score
HBCDD	422	0.74
TBECH	180	0.50
TCEP	117	0.34

B scores

The B scores are calculated using Equation 2. The equation uses the bioaccumulation factor, BAF as input. The equations below can be used to calculate the BAFs.

$$BAF_{birds,mammals} = TMF * BCF_{metabolism\_corrected} \qquad \text{Eq.12}$$

In which:
TMF = Trophic Magnification Factor
BCF = Bio Concentration Factor (=19673, EPIWIN).

The TMF is calculated according to equation 13 as following (Rorije et al., 2011).

$$TMF = -0{,}753 * (\log K_{oa})^2 + 13 * \log K_{oa} - 46{,}2 \qquad \text{Eq.13}$$

For HBCDD, TBECH and TCEP Koa and BCF input values come from EPIWIN. The used Log Koa, TMF and BCF values and the resulting B scores are presented in Table 45. The highest B score is for HBCDD, followed by TBECH. The B score for TCEP is approximately zero.

Table 45: Pov and B scores for HBCDD, TBECH and TCEP

Substance	Log Koa	TMF	BCF	BAF	B score
HBCDD	10.5	7.3	19673	52374	0.94
TBECH	8.0	9.6	18200	5647	0.54
TCEP	5.3	1.6	11	12	≈ 0

T scores

The T scores are calculated using Eq. 3 presented in the methodology chapter. The equation uses an estimation of the PNEC for the water compartment expressed in µg/l. The used PNEC values and the resulting T scores are presented in Table 46.

The largest change in the T score will occur at PNEC values in the range of 0.1-10 µg/l.

Table 46: PNECs (µg/L) and T scores for HBCDD, TBECH and TCEP

Substance	PNEC (µg/L)	T score	Remark
HBCDD	0.31	0.89	PNEC from EC (2008)
TBECH	4	0.17	Lowest NOEC/10 (40 µg/L /10) Nitocra spinipes (Nyholm, 2009)
TCEP	65	0.01	PNEC from EC (2009)

According to this assessment HBCDD is the most toxic. For the alternatives, the T scores are much lower.

Calculation of the overall PBT score

The overall PBT score is calculated by adding the P score, B score and the T score (Table 47).

Table 47: P, B, T and overall scores for HBCDD, TBECH and TCEP

Substance	P score	B score	T score	Overall score
HBCDD	0.74	0.94	0.89	2.57
TBECH	0.50	0.54	0.17	1.21
TCEP	0.34	≈ 0	0.01	0.35

In the case of HBCDD, the PBT score equals 2.57 and is closest to the maximum score of 3. Ranking the three substances according to the PBT potential, HBCDD is the highest, followed by TBECH and TCEP (Table 47). In addition, when looking to Table 47, it can be noticed that the B score of TCEP is very low, so it is likely that TCEP is not bioaccumulative. The substance is, however, persistent, but not toxic. On the basis of the alternative T score, the same overall conclusion can be drawn though one combination of high individual scores for instance high B score and high T score may be more or less relevant than a combination of a high P and T score. For the three substances considered the conclusions remain the same though.

1.4.2 *Step 4c: Environmental impact assessment based on the 'probabilistic' approach*

Calculation PAFs

The risk can be expressed by the RCR (PEC/PNEC) as is done section 1.2.3. Risks can be turned into impacts by the calculation of the percentage potentially affected species (PAF). For the PAF assessment a PEC (or a distribution of PECs) is needed that can be inserted into the formula (Eq. 14) to calculate the PAF. This formula integrates the hazard data as following:

$$PAF_{sub} = \frac{1}{1 + e - \dfrac{\log PEC_{reg,sub} - \alpha_{sub}}{\beta_{sub}}} * 100\% \qquad \text{Eq. 14}$$

PAFsub = Potential Affected Fraction
PECreg,sub = Regional Predicted Environmental Concentration of substance
α sub = average of toxicity data of substance
βsub = standard deviation of toxicity data of substance

Table 48: Calculated PEC and PAF values of HBCDD and TBECH for the various situations required to calculate the various Policy Scenarios considered within this case study

Substance	Scenario	PEC regional (mg/L)	PAF_regional (%)
HBCDD (all applications entire life-cycle)	BAU	$3,2.10^{-6}$	0,16
HBCDD (all applications entire life-cycle - EPS)	PS	$2,1.10^{-6}$	0,125
HBCDD (solely EPS)	PS	$1,1.10^{-6}$	0,084
TBECH (solely EPS)	PS1	$1,4.10^{-7}$	0,00067

BAU = HBCDD (all applications entire life-cycle - EPS) + HBCDD (solely EPS)
PS1 = HBCDD (all applications entire life-cycle - EPS) + TBECH (solely EPS)
PS2 = not performed
PS3 = HBCDD (all applications entire life-cycle - EPS)

As can be seen from the above table, the PECs are very low. Also, the calculated PAFs are low. Underneath, the numbers are used within the various Policy Scenarios.

PS1. Replacement of HBCDD within EPS with BTECH.

This scenario means that the effect is calculated by looking at the total effect of HBCDD (all applications entire life-cycle minus EPS) and the effect of the use of TBECH for solely EPS. For this scenario, the PAF needs to be calculated using a combiPAF according to Eq. 15 (Bakker and Van de Meent, 1997).

$$CombiPAF = 1 - (1 - PAF_{HBCDD,allapps-EPS}) * (1 - PAF_{TBECH,EPS}) \qquad \text{Eq.15}$$

The combiPAF of the use of TBECH within EPS (instead of HBCDD) is 0,126 and is 21,3% lower compared to the BAU scenario.

PS2. Replacement of HBCDD within EPS with TCEP

For this scenario, no PAF has been assessed. TCEP is solely used to test the PBT ranking methodology.

PS3. Replacement of EPS by another product that does not contain HBCDD or TBECH.

For this scenario, it means that the effect is calculated by considering the PAF of all applications’ entire life-cycle minus the PAF of all applications except EPS. The replacement of EPS with another product means that the PAF decreases from 0,16-0,125 = 0,035. The decrease compared to the BAU scenario equals 78,1%.

1.5 Step 5: Uncertainty analysis

1.5.1 Overview of sources of uncertainty and error in the end results

In these scenarios, different choices and assumptions have been made and also different input data are used and processed in different testing methods, equations and models. All these aspects can cause uncertainty or error to the end results. The table below (Table 48) gives an overview of the main sources of uncertainty and error of both the BAU and Policy Scenario and tries to indicate the possible effects of this on the end results/conclusions of the case study. The choice of the alternative and the used release estimations are indicated as the most relevant sources of uncertainty. Other relevant sources of uncertainty were the lack of hazard data and connected to that the choice of relevant endpoints. Besides that, the ignorance of the trend and the time span used were indicated as sources of uncertainty of with the relevance or influence could not be specified. Whether all indicated sources of uncertainty overall will cause an under- or overestimation of the results is unclear.
Note that this uncertainty table was not developed on the basis of expert elicitation. It was developed by one expert and checked by a second expert. The reliability of this uncertainty table could therefore be questioned and could be improved using expert elicitation.

Table 48: Overview of sources of uncertainty and error in the end results

Choice/assumption/input data used	Quantitative or qualitative description BAU	Quantitative or qualitative description PS	Validity	Consequence for the result[4]	Data source used and cause of uncertainty
Scope and scenario definition (choices and assumptions)					
(alternative) substance	HBCDD	TBECH; TCEP and non-EPS alternative are only included as alternatives that have partly been included in the assessment for methodology testing purposes	There is discussion on the validity of TBECH as alternative because of uncertainty on its technical feasibility. Other non-EPS alternatives might be more valid, but are not fully included in the assessment	**Relevant** source of uncertainty, score: 5 If non-EPS alternative would be included, toxicity of the PS might be significantly lower than TBECH. The environmental improvement in terms of ecotoxicity of the restriction could then increase and end result would thus be underestimated: --. If other (brominated) flame retardants would be included as alternatives the results could be either under or over estimated: ?	ECHA, 2009a RME, 2011
Replacement ratio alternative (degree of fire resistance)	Assumed is HBCDD:TBECH of 1:1		Assumption not based on anything due to lack of data. This assumption might not be valid.	Thought to have an impact on the final result and thus might be relevant: 2. Degree is uncertain, but could be better estimated using quantitative sensitivity analysis.	NA
Ignoring increasing use trend	Ignored	Ignored	Not valid as HBCDD is placed on Annex XIV of REACH	Impact on the results is uncertain as at this moment it is unclear what the effect of the listing on Annex XIV will be on the use of HBCDD and its alternatives. **Uncertain whether it is relevant** and uncertain what the consequence on the end results will be: ?	Annex XIV, REACH
Included life cycle stage: Formulation Industrial use Professional and private use Service life stages	Releases from literature	Releases from literature	Estimations reported in literature and are assumed to be valid	As all relevant life cycle stages are included for both BAU and PS, this source of uncertainty is not assumed to be very relevant: 1	ECHA, 2009a
Geographical scale	EU	EU	Valid	Expected to have minor influence. Relevance: 1	NA

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[4] Scoring based on expert judgement: 1 = low relevance, 5 = high relevance

Choice/assumption/input data used	**Quantitative or qualitative description BAU**	**Quantitative or qualitative description PS**	**Validity**	**Consequence for the result**[4]	**Data source used and cause of uncertainty**
Starting point in time of restriction	2006 is taken as the base line for use quantities	From 2007 onwards	NA	No source of uncertainty for this case study. Relevance: 1	NA
Included time span of effect	The effect is assumed to occur directly after emission/exposure	The effect is assumed to occur directly after emission/exposure	Not valid assumption, especially because we are dealing with materials that can have life spans of <50 years and because we are dealing with a PBT (BAU) and a likely persistent/bioaccumulating substance (PS), and thus impacts will likely occur years/decades after use and exposure	Is expected to be a relevant source of uncertainty, especially if effects are to be discounted over time (e.g., in SEA context). In comparing BAU and PS the ignorance of the time span might be relevant to some extend as possible effects of PS are expected to occur earlier in time then of BAU. **Depending of the discount rate chosen this source of uncertainty will be more or less relevant.** The end result might in any case be overestimated: +	NA
Assumed trend in use (import, export, production)	No trend assumed, one reference year taken	No trend assumed, same reference year taken as for BAU	Not valid since available data shows an increase in use of EPS	Source of uncertainty is not assumed to be very relevant: 1. The ignorance could cause an underestimation of the results: -	Ignored
Choice of relevant ecotox endpoints	Toxic and PBT	Lack of data but indicated as P and B (TBECH and TCEP)	Valid as far as data is available	**Expected to be relevant**: 4. Due to lack of data on the PS, not all relevant endpoints might be included. End result might be under- or overestimated: +/-	EC (2008), ECHA (2009a), EpiSuite, ECOSAR
Choice of relevant environmental compartments	Aquatic and lipid (secondary poisoning)	Aquatic and lipid (secondary poisoning)	Soil/sediment ignored	Expected to be relevant as soil/sediment are expected to be relevant: 3. Final result may be under- or overestimated: +/-	Ignored
Input data and model/parameter uncertainties					
Included use amounts	5301/5652 tonnes	5301/5652 tonnes	See assumed trend in use	Assumed to be equal for BAU and PS (See assumed trend in use), relevance: 1	See assumed trend in use
Release estimation (Air Water (surface	Assumed that use = release	Assumed to be the same as for HBCDD: use = release	Uncertain	**Highly relevant**; 5; possible over- or underestimation of the results, as not all amounts used might be emitted both for	ECHA (2009a) for HBCDD, for TBECH and TCEP

Choice/assumption/input data used	Quantitative or qualitative description BAU	Quantitative or qualitative description PS	Validity	Consequence for the result[4]	Data source used and cause of uncertainty
water), Soil).				BAU and for PS.	assumptions
PEC estimation	Based on EUSES calculation (P/C properties and release data)	Assumed to be similar to BAU	Assumption of similar release between BAU and PS is uncertain	Highly relevant**:** 5; however, already expressed under ‘release estimation’.	Assumptions
Hazard data, included species	Fish, Algae and Daphnia (HBCDD)	Fish, Algae, Daphnia and Nitocra spinipes (TBECH). TCEP NA	For PS lack of experimental data, therefore QSARs were used. This increases the uncertainty on the PS.	**Relevant impact on result**: 4. PNECs (especially for PSs) might be over- or underestimated: +/-	EC, 2008, ECOSAR
Used assessment/extrapollation factors	Ignored	PS for secondary poisoning an assessment factor of 30 was applied	Lack of data	Relevant for secondary poisoning: 3. Might cause under- or overestimation: +/-	EC, 2008
Used physical-chemical property data (molecular weight, melting point, vapour pressure, water solubility, octanol-water partition coefficient	Used as input into EUSES with release factors to calculate PECs	Used as input into EUSES with release factors to calculate PECs	Valid	Relevant: 2; but limited influence on the PEC compared to the influence of the used releases	EC, 2008, online chemical database(s)
Fate and distribution factors BCF and BMF	Used as input into the calculation of the RCRs and PBT scores	Used as input into the calculation of the RCRs and PBT scores	Valid	Relevancy: 4 for RCR score. Relevancy: 4 for PBT score.	Calculation based on numbers generated by EPIWIN

1.6 Step 6: Comparison of the scenarios

In this case study, the environmental impact of the replacement of HBCDD within EPS has been assessed in terms of the potential affected fraction (PAF) and PBT ranking scores. Where it was not possible to come to an indication of the potentially disappeared fraction of species, the risk characterization ratio was the resulting indication to be used.
In total, two main scenarios were set up that each had its specific assumptions; the Business As Usual (BAU) scenario and the Policy Scenario (PS). The BAU scenario assumed that everything would remain the same and the PS assumed that the use of HBCDD for EPS was restricted. For the PS, three sub-scenarios were created in which it was assumed that HBCDD was replaced by two alternatives, being TBECH (PS1) and TCEP (PS2). TCEP was solely used within the testing of the PBT ranking methodology; no PAF was calculated for this scenario. The third scenario assumed that the product EPS was replaced by another product not containing (and requiring) a flame retardant.

Before comparing the scenarios, it should be mentioned that this case study had to deal with a serious lack of data. At the international level, discussions are still ongoing about whether technical feasible alternatives of HBCDD in EPS are available, and consequently the feasibility of TBECH is discussed as well. It is uncertain whether the alternatives included in this case study are realistic alternatives in practice. For the two alternatives that were included, very few toxicity data were found, and due to a complete lack of production, use and release data of TBECH, these data have been assumed to be the same as those of HBCDD. This indicates the largest drivers of the total uncertainty within this case study: the choice of the alternatives, the release or emission estimates used. The uncertainties caused by the lack of hazard data are assumed to be of lower importance. As indicated in the uncertainty table, other sources of uncertainty can also have influence on the end results. Whether the indicated sources of uncertainty would imply an overall under- or overestimation of the end results could not be specified. Neither could be indicated what the actual consequence of the uncertainties on the end conclusion could be.

As we are dealing with at least one PBT substance, the overall assessment was based on PBT scoring, and additionally a targeted impact assessment based on secondary poisoning and on the water compartment was applied.
Both the individual P, B and T scores and the total PBT score show similar trends when comparing BAU (HBCDD) to PS1 (TBECH) and PS2 (TCEP). The scores for HBCDD are all relatively high compared to the scores of the other substances reviewed (0.74, 0.94, 0.89 and 2.57), indicating HBCDD to be a substance that is very persistent, bioaccumulative and toxic. For TBECH, the scores are all around average (0.50, 0.54, 0.17 and 1.21), indicating that the substance is less persistent, bioaccumulative and toxic. TCEP shows even lower scores for all indicators (0.34, 0, 0.01 and 0.35). This substance proves to be somewhat persistent but has a very low bioaccumulation or toxicity potential compared to HBCDD and TBECH. On the basis of the PBT scoring, only replacement of HBCDD with TBECH implies an substantial environmental improvement and replacement with TCEP an even larger improvement.

However, the PBT scoring does not include exposure estimates and does not tell anything on actual expected impacts (and thus on actual levels of improvement).For this reason the impact assessment was added. Unfortunately, no potentially disappeared fraction of species could be derived for secondary poisoning, due to the lack of hazard data. For secondary poisoning, we thus only

have the RCR values indicating a risk for BAU (RCR = 22.2) and no risk for PS2 (RCR ≈ 0). No risk indication could be derived for PS1.
For the aquatic compartment, an impact indication was made resulting in a potentially disappeared fraction of species of 0.16 for BAU and 0.125 for PS1 (an improvement compared to BAU of around 21%). PS3 would result in a PAF of 0.035 (an improvement compared to BAU of around 78%). Although relative improvements are substantial, the absolute improvements are only marginal. Thereby, the impacts calculated for the water compartment are of limited relevance with regard to this case study, as the major concern of PBT substances are found in their probable accumulation into lipids and thus into the food chain (or into soil and sediment).

In summary, reviewing the RCRs, PAFs and PBT scores of BAU, PS1 and PS2 shows that both PS1 and PS2 show an improvement compared to BAU, both in terms of RCRs and PAFs and in terms of PBT scores. The level of improvement could unfortunately not be defined.

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Erratum on report 601353002 (2012): From risk assessment to environmental impact assessment of chemical substances, methodology development to be used in the socio-economic analysis for REACH

In chapter 6 on page 77 the reference to RPA (2010) is incorrectly stated. The correct reference is:
RPA, 2011. Assessing the Health and Environmental Impacts in the Context of the Socio-economic Analysis Under REACH. Part 1: Literature Review and Recommendations and Part 2: The Proposed Logic Framework and Supporting Case Studies.
ENV.D.1/SER/2009/0085r. Final Report.

In Appendix A, section 1.1 the first bullet under part B is incorrectly published and should be deleted ('- Relevance: ……… measure under study').

Appendix D, section 1.1.2 on page 138 states: 'ECHA estimated the total use of HBCDD about 11 tonnes/year in 2006 (ECHA, 2009a). Since 5.3 tonnes were used for EPS in 2006 this equals about 45% of the total HBCDD use.' The units presented in these sentences are incorrect, and should be 11 ktonnes and 5.3 ktonnes, respectively.

In Appendix D, section 1.2.3 on page 142, table 42 has accidentally not been published. The table is presented below.

Table 42: Overview of toxicity data for aquatic species for the determination of the species sensitivity distribution function (SSD)

Species per substance	Duration	Type	Concentration (mg/L)	Method[1]
HBCDD				
Fish	14-day	LC50	0.606	Calc.
Green Algae	96-hr	EC50	0.199	Calc.
Daphnid	16-day	EC50	0.065	Calc.
Skeletonema costatum		EC50	0.052	Meas.[2]
Fish	30-day	ChV	0.043	Calc.
Thallassiosira guillardii	72-hr	EC50	0.04	Meas.[3]
Daphnia magna	21-day	NOEC	0.0031	Meas.[4]
Average (mg/L), α			-1.0	
Standard deviation, β			0.7	
TBECH				
Fish	14-day	LC50	0.865	Calc.
Fish	30-day	ChV	0.062	Calc.
Green Algae	96-hr	EC50	0.288	Calc.
Daphnid	16-day	EC50	0.081	Calc.
Nitocra spinipes	96-hr	NOEC	0.04	Meas.[5]
Average (mg/L), α			-0.9	
Standard deviation, β			0.5	

Note that for this case study different hazard endpoints (LC50, EC50, ChV and NOEC) were combined in the SSDs. This was done for reasons of data shortage, to be able to perform this part of the impact assessment as an exercise. However, note that from a scientific point of view, it is not correct to combine different hazard endpoints into one SSD.
Note 1: calc. values calculated by ECOSAR model (US-EPA, 2004); meas. Values based on measured toxicity data
Note 2,3, 4: data taken from EC (2008)
Note 5: Nyholm (2009)

In Appendix D, section 1.2.2 on page 141 a reference to table 8 is incorrectly stated. The correct reference is table 41.

Appendix D, section 1.5.1 pages 148 and 149 show table 48 and a reference to table 48. In both cases the correct table number is 49.

For agreement, 19 June 2012

Dr. J.M. Roels
Head Expertise Centre for Substances
RIVM

National Institute for Public Health
and the Environment
P.O. Box 1 | 3720 BA Bilthoven
www.rivm.com