LIFE / FIT FOR REACH

Environmental indicator concept

2016

The Project "Baltic pilot cases on reduction of emissions
by substitution of hazardous chemicals and resource efficiency"
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Contents

Abbreviations

ALO:	Agricultural Land Occupation
AoP:	Areas of Protection
CC:	Climate Change
CCR:	Change in Chemical Risk
CMR:	Carcinogenic, mutagenic, reprotoxic
ConsExp:	Consumer Exposure model
DMEL:	Derived minimal effect level
DNEL:	Derived no effect level
DPSIR:	Drivers, Pressures, State, Impact, Response
EC:	European Commission
ECETOC TRA:	Ecetoc targeted risk assessment
EEA:	European Environment Agency
EIA:	Environmental Impact Assessment
Env.:	Environment
ERC:	Environmental Release Categories
EU:	European Union
EUSES:	European Union Substance Evaluation System
FD:	Fossil Fuel Depletion
FE:	Freshwater Eutrophication
FET:	Freshwater Ecotoxicity
HH:	Human health
HT:	Human Toxicity
IR:	Ionising Radiation
LCA:	Life Cycle Assessment
LCI:	Life Cycle Inventory
LCIA:	Life Cycle Impact Assessment
LCT:	Life Cycle Thinking
ME:	Marine Eutrophication
MET:	Marine Ecotoxicity

MRD :	Mineral Resource Depletion
NLT :	Natural Land Transformation
NMVOC:	Non-methane volatile organic compounds
OD :	Ozone Depletion
ODS:	Ozone Depleting Substances
PBT:	Persistent, bioaccumulative and toxic
PEC:	Predicted environmental concentration
PM:	Particulate Matter
PMF:	Particulate Matter Formation
PNEC:	Predicted no effect concentration
POF:	Photochemical Oxidant Formation
RA:	Risk Assessment
RCR:	Risk characterisation ratio
REACH:	Registration, Evaluation, Authorisation and Restriction of Chemicals
SCP:	Sustainable Consumption and Production
spERC:	Specific Environmental Release Category
SVHC:	Substances of Very High Concern
TA:	Terrestrial Acidification
TET:	Terrestrial Ecotoxicity
ULO:	Urban Land Occupation
UNEP:	United Nations Environment Programme
VOC:	Volatile Organic Compounds
vPvB	Very persistent, very bioaccumulative
WD:	Water Depletion

1. Aim of indicators

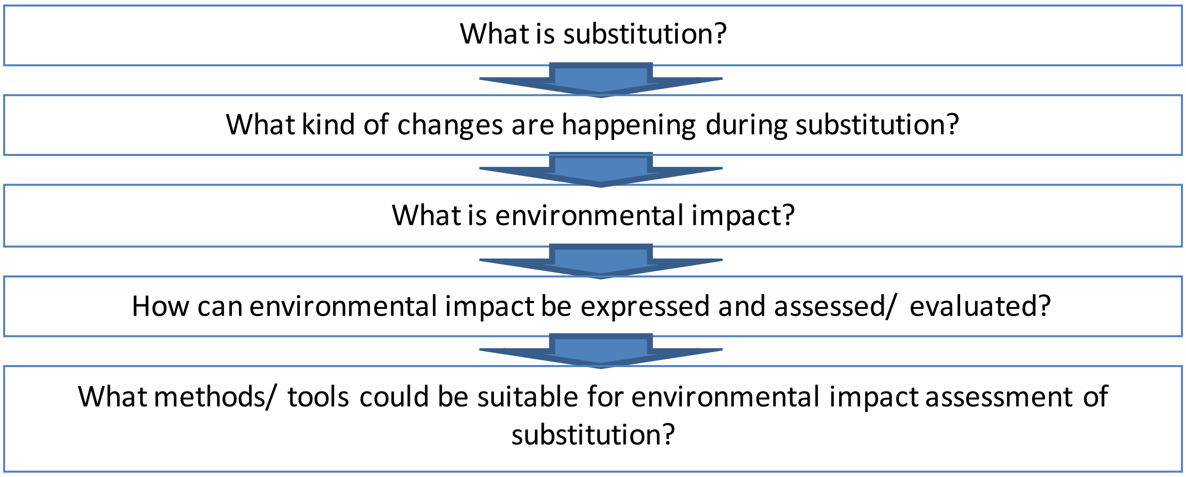
The task of Action C1 of the project Fit for REACH is environmental impact assessment, i.e. it aims to evaluate changes achieved due to a substitution / resource efficiency measures and to hence illustrate the contribution of companies / the project to the improvement of the environmental state:

$$\Delta_{\text{env imp}} = \text{Impact}_{\text{initial}} - \text{Impact}_{\text{after the substitution}}$$

The task of Environmental Indicator Concept is to propose how to calculate this equation, i.e. to propose indicators that represent environmental impact of substitution / resource efficiency measures[1].

2. Overview

In order to propose indicators and to assess environmental impact of a substitution, it is needed to clarify:



2.1 What is substitution?

Substitution means “replacing hazardous substances in products and processes by less hazardous or non-hazardous substances, or by achieving an equivalent functionality via technological or organisational measures” (EC, 2003). It is at the top of the hierarchy of control measures applied to substances or mixtures, meaning that a greatest value is on hazard avoidance, not exposure controls.

The EU REACH regulation calls for the substitution of the most hazardous substances, called **S**ubstances of **V**ery **H**igh **C**oncern (SVHC). These are substances which are **C**arcinogenic, **M**utagenic and **R**eprotoxic (CMR) or which are **P**ersistent, **B**ioaccumulative and **T**oxic (PBT) or **V**ery **P**ersistent and **V**ery **B**ioaccumulative (vPvB) or have other properties giving rise to an equivalent level of concern (e.g. endocrine disruptors or respiratory sensitisers). Also other legal acts stipulate substitution (e.g. carcinogens and mutagens shall be substituted according to Carcinogens and Mutagens Directive (2004/37/EC)). Less hazardous substances may also be replaced, since substitution is a general recommendation.

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[1] According to the definition given by the European Environmental Agency, an environmental indicator is an observed value representative of a phenomenon under study (EEA, 1999).

2.2 What changes are happening during the substitution?

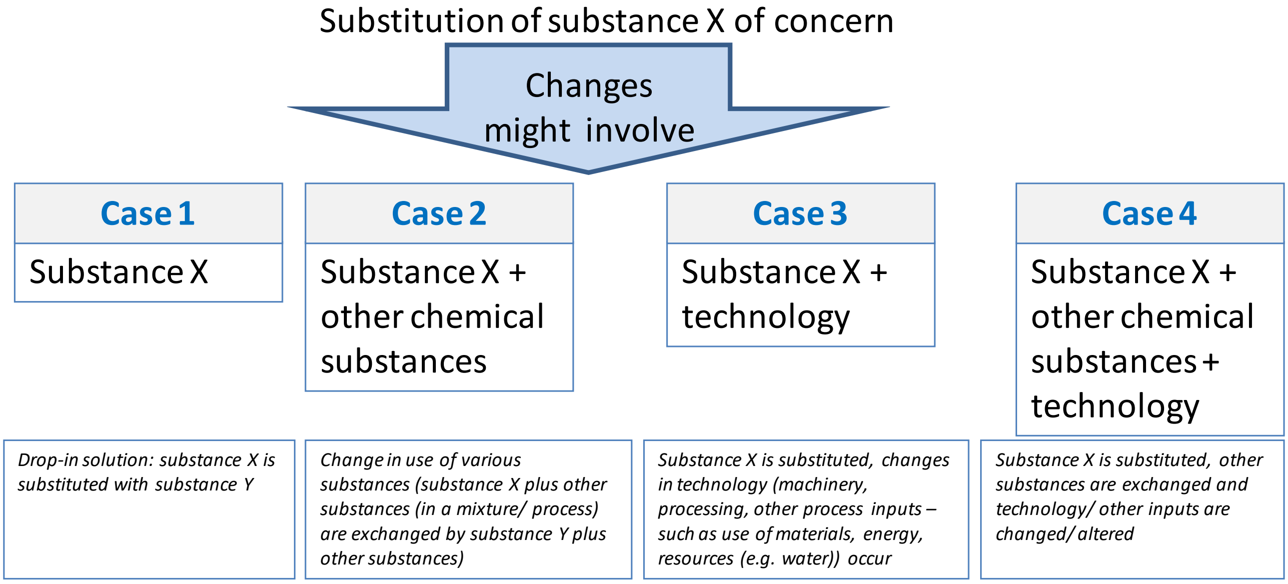
Substitution might be implemented in a number of ways:

- using different and safer[2] substance(s) instead of the initial one or fully omitting it, without or with change in technology;
- using a (non-chemical) technological alternative or organisational measure instead of the initial substance.

It is the core aim of substitution to eliminate or reduce the use of hazardous substances. The chemical of interest and its alternatives may pose hazard to human health or to the environment or to both, as well as cause different effects to humans or the environment (e.g. neurotoxicity vs. respiratory sensitization). A focus on a key property, e.g. the one triggering the substitution (e.g. CMR or high chronic toxicity to the aquatic environment) would prevent identification of all potential risks to humans or the environment; hence, all hazards (and exposures) should be considered to evaluate a substitution process with regard to the change in chemical risk.

Also, it is needed to consider other environmental impacts than chemical risks. Excluding them could lead to a wrong estimation of an overall environmental impact. Substitution of the target hazardous substance by an alternative substance might be accompanied by changes in e.g. energy or water consumption, which may be either beneficial for the environment or cause an additional pressure.

The complexity of substitution cases is illustrated in Fig. 2.1.



Drop-in solution: substance X is substituted with substance Y

Change in use of various substances (substance X plus other substances (in a mixture/ process) are exchanged by substance Y plus other substances)

Substance X is substituted, changes in technology (machinery, processing, other process inputs – such as use of materials, energy, resources (e.g. water)) occur

Substance X is substituted, other substances are exchanged and technology/ other inputs are changed/ altered

Fig. 2.1. Complexity of substitution, showing changes that might be triggered by substitution of the hazardous substance of concern.

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[2] Unfortunately, substitution could also be implement using less safe chemicals, not because people want it but because they don't know better (lack of information – so called regrettable substitution)

2.3 What is environmental impact?

Definition of environmental impact is presented in various contexts/ documents:

- Life cycle assessment defines environmental impact as a consequence of an environmental intervention in the environment system; environmental intervention – a human activity affecting the environment, either physical, chemical or biological; in particular resource extraction, emissions and land use (CML et al, 2001).
- EIA (environmental impact assessment) Directive (2001/92/EU) defines environmental impact in the wider context, i.e. directed towards the development projects. Environmental impact - any change in the physical, natural or cultural environment brought about by a development.
- UNEP report "Assessing the environmental impacts of consumption and production" defines environmental impacts as the unwanted by-product of economic activities (UNEP, 2010).

Other sources present similar definitions. To summarize them, that is the effect that the activities of people and businesses have on the environment.

2.4 How can environmental impact be expressed and assessed/ evaluated?

Types of environmental assessments can be grouped based on various criteria: scope (broad environmental outlook, thematic assessment), scale (global, regional, national, and corporate), purpose (demonstrate the benefits of policy options or decide upon the need to modify them, legally required assessment of planned projects (EIA, SEA)), target group (policy makers, companies, society). Environmental indicators are being used in environmental assessments to aggregate environmental information into parameters representing a certain type of effect, thus making complex phenomena more obvious and potentially measureable (over time).

There is a number of methodologies used in environmental assessments and allowing to calculate/ estimate the chosen environmental indicators. The OECD developed a set of harmonised international environmental indicators (OECD, 2003). It proposed a framework – Pressure – State – Response model – for grouping indicators. The DPSIR framework (Driving forces, Pressure, State, Impact, Response) was proposed to be used by European Environment Agency in its reporting activities (EEA, 1999) (Fig. 2.2). This grouping helps for the general understanding of origins and consequences chain:

driving forces and	*Indicators for driving forces describe the social, demographic and economic developments in societies and the corresponding changes in life styles, overall levels of consumption and production patterns*
the resulting environmental pressures, on	*Pressure indicators describe developments in release of substances (emissions), physical and biological agents, the use of resources and the use of land.*
the state of the environment and	*State indicators give a description of the quantity and quality of physical phenomena, biological phenomena and chemical phenomena (such as concentrations of chemicals in the environment) in a certain area.*
impacts resulting from changes in environmental quality and on	*Impact indicators are used to show impacts on the social and economic functions on the environment, such as the provision*

	of adequate conditions for health, resources availability and biodiversity.
the societal response to these changes in the environment.	*Response indicators refer to responses by groups (and individuals) in society, as well as government attempts to prevent, compensate, ameliorate or adopt to changes in the state of the environment.*

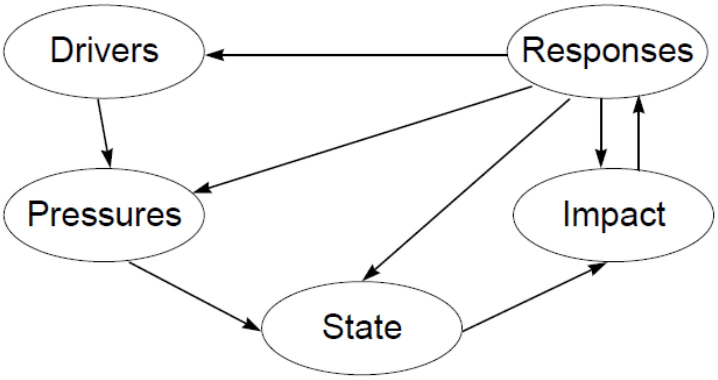

Fig. 2.2. The DPSIR Framework (EEA, 1999).

Environmental indicators that are suitable to be applied at corporate level for the evaluation of production processes and products can be classified into four main groups: 1) indicators of energy and material flows; 2) indicators with a territorial dimension; 3) indicators of Life-Cycle Assessment; 4) indicators of environmental risk assessment (Herva et al, 2011). Indicators and methodologies/ tools that are used to derive them are summarised in Fig. 2.3. There are examples when different tools are used complementary in order to achieve a desired picture of environmental situation (Herva et al, 2013; Kikuchi et al, 2011).

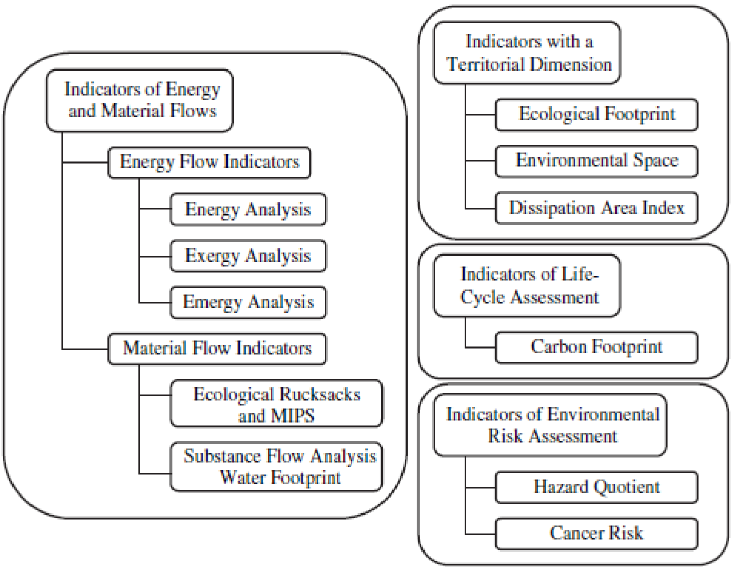

Fig. 2.3. Examples of environmental indicators at the corporate level (from Herva et al, 2001).

Of the mentioned tools, material and energy flows can be considered as the basis on which all other environmental evaluation tools and indicators are founded. Indicators like ecological[3] or carbon footprint are easy to understand by various stakeholders. Nevertheless, due to highly aggregated nature they lose ability to provide specific information. LCA is commonly regarded as the only methodology that provides a comprehensive assessment of the environmental impacts associated to an activity or product. But again, this broad perspective is a consequence of the inventory compiled rather than of the methodology itself: what system boundaries do we establish, what processes do we include.

Chemical risk assessment (RA) is the practice of estimating the severity and likelihood of harm to human health or the environment occurring from exposure to a chemical substance (or mixture). It is important to recognize that RA and alternatives assessment (although both share the same elements – hazard and exposure assessments, with the alternatives assessment evaluating the technical and economic feasibility of the use of a substance in a particular application) are intended to perform different functions. RA answers the question "Is this chemical or product safe enough for the intended use?" in contrast to an alternatives assessment, which is intended to answer the question: "Which chemical or product is a safer choice for the use?" (Wittaker, 2015). The assessment of (changes in) chemical risks is crucial in the evaluation of substitution of chemicals, as the core aim of substitution is to eliminate or at least reduce a chemical risk as much as possible.

An assessment of environmental impacts could be a part of an alternatives assessment. Nevertheless, alternatives assessment not only looks at changes in risk and/or environmental impacts but also at the technical feasibility of substitution (does the substitute fulfil its function, is it possible to apply in the process / product without decrease in quality) and at the economic side of the game – are the costs proportionate and which alternative has the best cost/benefit ratio). It needs to end-up in a decision taken on which substitute to choose.

2.5 What methods/ tools could be suitable for environmental impact assessment of substitution?

The different kinds of available methodologies and indicators can highlight different potential environmental problems, but none of them offers a comprehensive measure of the environmental impacts as a consequence of anthropogenic activities. The use of several complementary methodologies might be advantageous and should be the preferred option to obtain different perspectives and a wider approach of the analysis carried out.

Material and energy flows can be considered as the basis on which all indicators are founded. They reflect the consumption of resources from nature and the emission of pollutants to the environment. These flows can be considered separately (e.g. input-output of a chemical substance X of concern, and input-output of other related substances), certainly providing more detailed information, or aggregated, thus reducing the number of indicators to be handled (e.g. emissions of substances having PBT properties, or even more aggregated – e.g. risk or toxicity from substance X of concern and other related substances).

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[3] The Ecological Footprint represents the productive area required to provide the renewable resources humanity is using and to absorb its waste. It measures the "quantity of nature" that we use, and compares it with how much we have (biocapacity). http://www.footprintnetwork.org/en/index.php/GFN/

A strong link exists between material and energy flows and LCA, since inventories used for material and energy flows are generally based on a life-cycle perspective. However, material and energy flows reveal pressures, but do not evaluate impacts on human health and environment. So they are not exchangeable, but can complement each other. In our case, material and energy flow analysis can show what is the usage (inputs) and emissions of chemical substance X of concern and other related chemicals or materials / resources/ energy, and what are emissions (outputs) at certain stages of life cycle. This information can then be „translated“ into environmental impacts in the form of environmental impact assessment categories, and also into risk to human health and environment.

LCA is claimed to offer an integrative assessment of a process. In our case, we can use LCA to evaluate environmental impacts from emissions of a substance X of concern + other related chemical substances + other changes in the process as a result of substitution. However, it is done for the regional or global level. Risk assessment has been developed particularly to account for toxicological and ecotoxicological risks caused by chemical substances, and it allows assessment for the environment at local level (short – term) and regional level (long-term) and for workers and consumers regarding acute exposures and long-term exposure. It allows account for different scenarios and events, distribution and transfer routs, exposure pathways, duration and frequency of the events.

3. The used indicator system

3.1 The proposed environmental impact indicators

The proposed environmental impact indicators are summarised in Table 3.1. They are explained further in the text.

Table 3.1. The proposed environmental impact indicators

DPSR framework stage	Indicator	Default / custom	Indicator levels		Method used	What is covered/ assessed with an indicator?
			Project level	Company level		
Pressure	**Emissions of target substances**	Default	kg/year of substance emitted	kg/year of substance per company	Emissions estimated using spERCs	Substitution of the substance of concern
		Custom	kg/year of: • PBT/vPvB; • CMR; • Other[4] for all companies – project partners;	kg/year per substance group per company		
State	Change in **environmental impact category indicator** values: - Toxicity; - Ecotoxicity; - Photooxidant formation; - Global warming; - Resource depletion; - ...	Custom	Sums within different environmental impact categories of the changes at the level of individual companies (recalculated per one year)	Change in environmental impact category results for functional unit	Life cycle assessment	Substitution of the substance of concern + change in other chemicals + other changes

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[4] In case of doubling of hazardous properties, substances are accounted in this way: PBT/vPvB > CMR > other

Impact	**Change of chemical risk**	Custom	Sums within different RCR types of the changes in RCR	Change in Risk characterisation ratio RCR (different types) per company	Chemical risk assessment	Substitution of the substance of concern + change in other chemicals
Response	**Substituted hazardous substances**	Default	kg/year of substance substituted	kg/year of substance per company		Substitution of the substance of concern
		Custom	kg/year of: • PBT/vPvB; • CMR; • Other[4] for all companies – project partners, and light case companies.	kg/year per substance group per company		

3.2 Reasoning

The choice of the proposed environmental impact indicators depends on:

1. the purpose of the indicators and/or the users of the indicators; i.e. should the indicators be used by project assessors to measure the overall success of the project (higher aggregation level) or should companies themselves measure their progress (higher level of detail).

There are two sets of interlinked environmental indicators in this project:

The “project indicators” should inform the project management and the project assessors about the overall environmental impacts of the project activities. The change is described by comparing the baseline situation when starting the project (before hazardous substances are substituted) with the situation at the project end (after substitution). The project indicators are derived from indicators developed at company level.

The “company indicators" should inform the project team and the companies carrying out a particular (substitution or resource efficiency) activity of the impacts of that activity (monitoring changes after an action is implemented).

2. the definition / scope of the environmental problem which is being tackled during the project / activities:

i.e. elimination/ reduction of emissions of hazardous chemical substances by substitution / resource efficiency measures;

in order to prevent bias, all aspects of the environmental problem that could be affected (to the better or worse) should be included to create a comprehensive picture;

Therefore the proposed indicator system:

- considers both ecotoxicological and toxicological hazards of chemicals (we look at humans as a part of the environment);
- covers a variety (complexity) of substitution cases;
- takes a life cycle perspective: substance X might be emitted and changes might take place not just during the production phase, but also later on in the life cycle of the product, e.g. during the use phase;
- covers local and regional/ global impacts;
- covers the relevant default indicators required by LIFE program.

The ability of the proposed environmental impact indicators to tackle various changes occurring as a result of substitution, to cover various life cycle stages and to deal with those affected (natural environment or humans (workers, consumers) is illustrated in Tables 3.2 and 3.3.

Table 3.2. Changes (occurring as a result of substitution) that are taken into the consideration by the proposed environmental impact indicators

Environmental impact indicators / **Changes occurring with:**	**Emissions of target substances** ***Default indicator***	**Change in chemical risk**			**Change in environmental impact category indicator values**	**Substituted target substances** ***Default indicator***
		Workers	**Users**	**Environment**		
Target substance	√	√	√	√	√	√
Other chemical substances		√	√	√	√	
Technology / other inputs					√	

Table 3.3. Life cycle stages that are taken into the consideration by the proposed environmental impact indicators

Environmental impact indicators / **Life cycle stages:**	**Emissions of target substances** ***Default indicator***	**Change in chemical risk**			**Change in environmental impact category indicator values**	**Substituted target substances** ***Default indicator***
		Workers	**Users**	**Environment**		
Production of inputs (chemicals, raw materials, energy)					√	
Production at company	√	√		√	√	√
Use	√		√	√	√	
Waste treatment					√	

The proposed environmental impact indicators represent pressures, environmental state (in other words – impact mid-points or impact categories), impacts (risk characterisation ratio), and response (see Fig. 3.1), this way covering the causal chain.

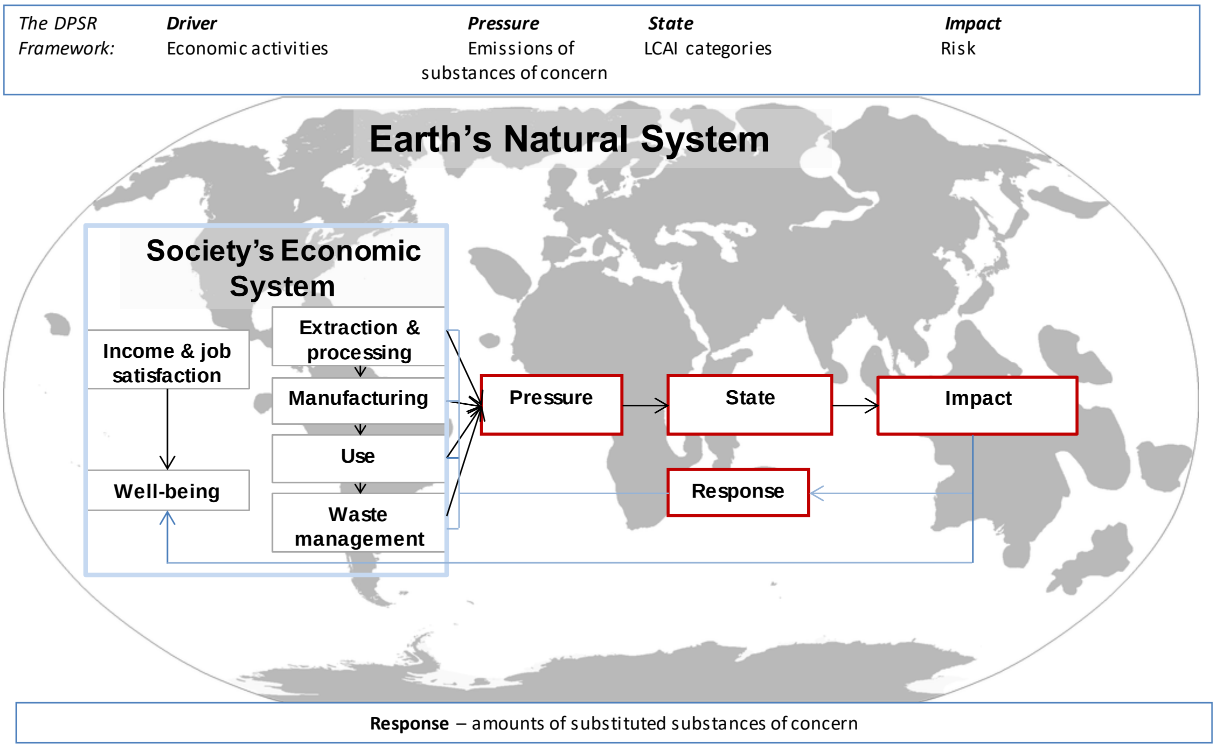

Fig. 3.1. Stages of DPSR framework, covered with the proposed environmental impact indicators (noted with red line).

3.3 Some remarks on the default LIFE indicators on chemicals

LIFE program presents some default indicators related to chemicals:

- emissions of target chemical substances at the beginning, at the end of the project, and 5 years beyond;
- substituted chemical substances (their amounts).

Both emissions of target chemicals and substituted chemical substances fit into the DPSR framework:

- emissions of chemicals show the pressure on the environment induced by the target substance,
- substituted chemicals show response to the issue.

It should be noted that the default indicators of the LIFE programme "substance emission" has a limited meaning with regard to environmental pressures and the respective state of the environment.

For persistent substances (PBT/vPvB), the emitted amount can be directly related to a pressure on the environment. Politically, precautionary approach is chosen to limit emissions of these substances to the environment because it is not possible to determine which emission / exposure level is not causing a risk (uncertainty about the substance hazards and uncertainties about exposure predictions).

Substances which might cause cancer, gene mutations or reprotoxic effects (CMR) might behave very differently in the environment. If they are rapidly degradable, they will not remain in the environment and have only a short time window within which they can cause damage. Other substances may not be degraded or destroyed quickly and they could therefore occur in relevant concentrations in the environment. However, whether or not they would cause any harm is unclear, because their toxic effects are determined only with regard to human health and not the environment.

The default indicator “PBT/vPvB emitted to the environment” is useful as environmental performance indicator. Due to the lack of meaning for CMR substances (and other substances), we included the Risk Characterisation Ratio (RCR) in our environmental indicator concept, which takes the environmental fate and behaviour of substances into account.

Even more, drop-in solutions when substance X of concern is exchanged with substance Y, which is not considered hazardous, and nothing else changes are uncommon. In order to get a comprehensive assessment of changes in environmental impact, it is important to take into account that other chemical substances having other (presumably less hazardous) properties will be introduced instead of the target substances; and/ or changes in technology (raw materials or energy) might occur. Thus, concentrating purely on emissions of target substances gives only a partial representation of environmental impact of substitution (see Table 3.2).

Additional environmental impact assessment indicators had to be proposed in order to be able to understand what kind of changes are occurring in the environment as a result of substitution.

3.4 Implementation of the environmental impact indicators

All the proposed environmental impact indicators shall be applied in case of the companies – project partners. Emissions of target substances and substituted amounts will be the major indicators in case of “light” case companies. Calculation of change in risk characterisation ratios and environmental impact category indicators will be implemented on case by case basis as these indicators require substantial amount of data and high degree of maturity of the case.

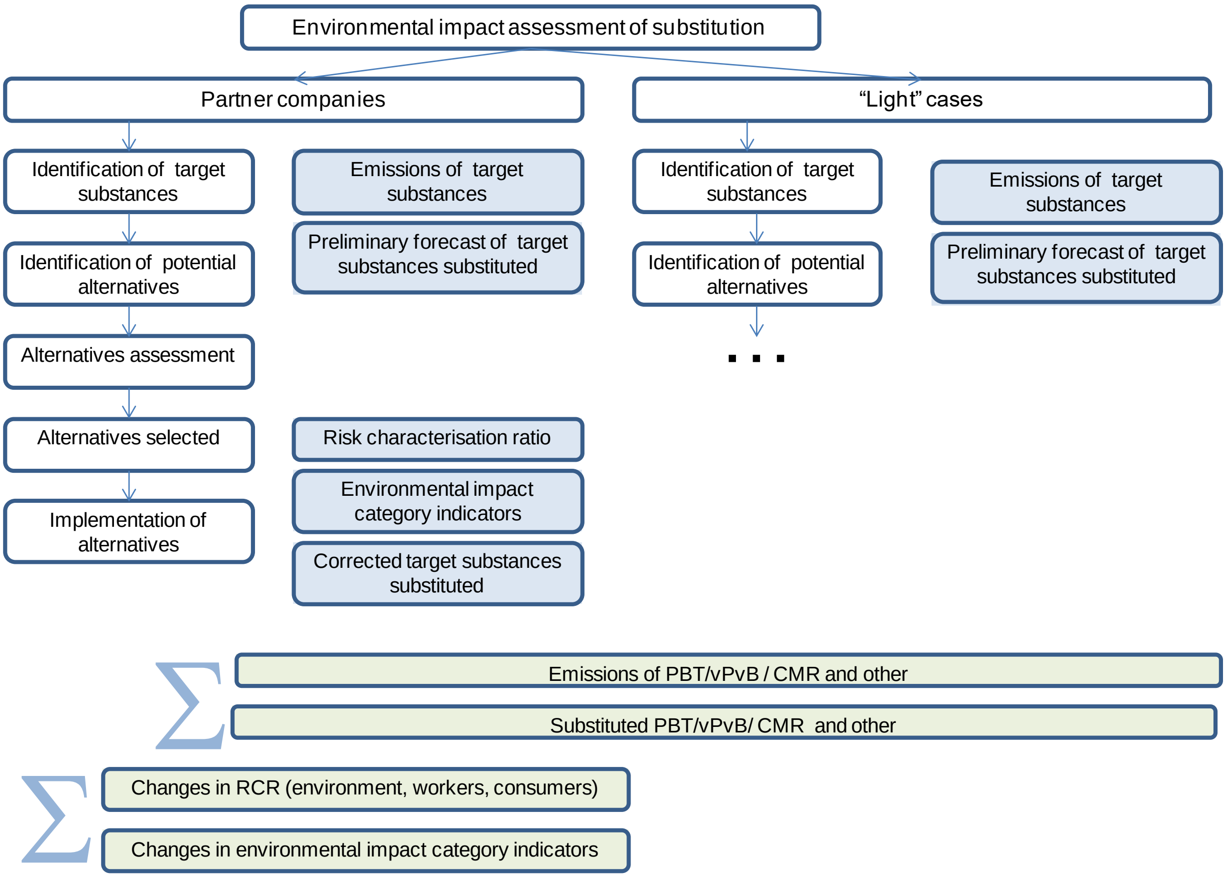

Fig. 3.2. Implementation of environmental impact assessment indicators.

Timing for application of indicators:

- Default indicators "emissions of target substances" and "substituted target substances" can be applied early in the process whenever substances of concern, which shall be substituted, are identified;
- Indicators "change in risk" and "change in environmental impact category indicators" can be applied only after the selection of alternatives, as these indicators take into the consideration not only target substances, but also other substitution related changes that must be known when performing risk assessment and / or life cycle assessment.
- Preliminary forecast of substituted substances shall be corrected by the end of the project.
- Quantification of indicators at project level is derived from indicators calculated at companies' level.

The scope for deriving indicators is the following:

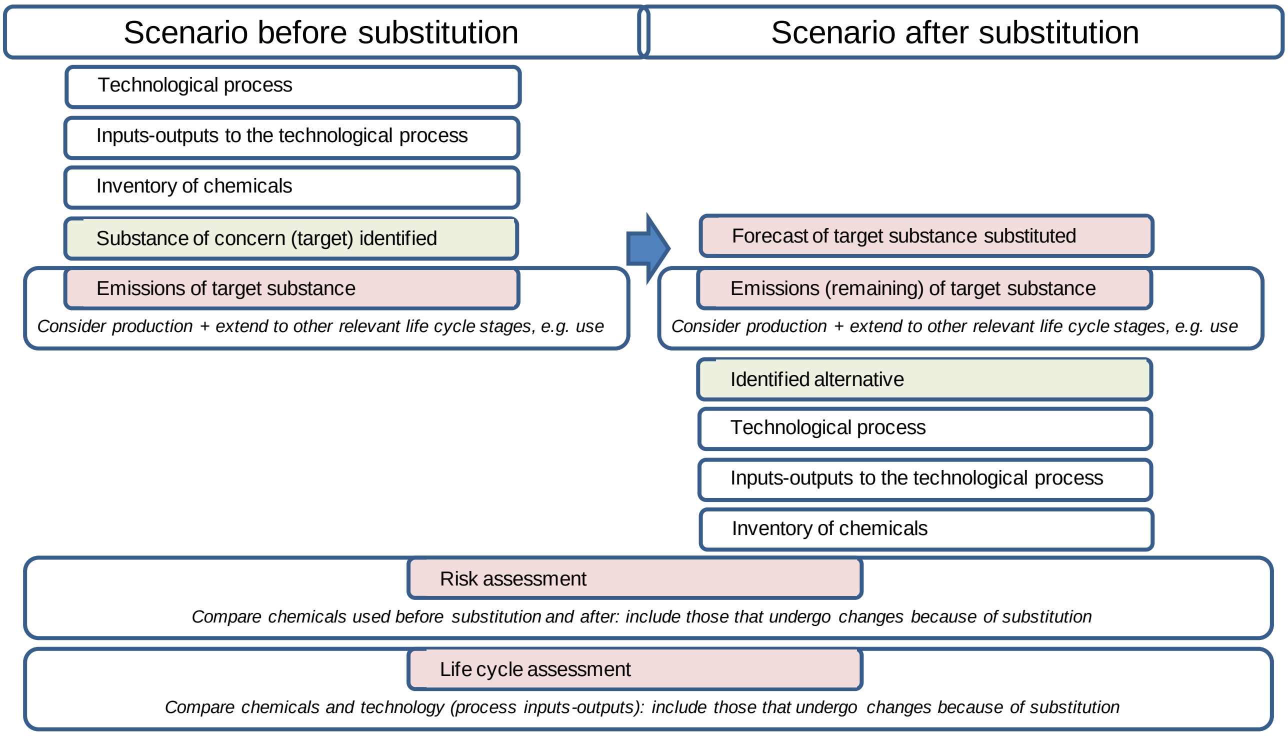

Fig. 3.3.

Technological scheme and a short description help to understand the process, which is subject for substitution.

The purpose of making input-output analysis, or, in other words, material and energy balance, is to account for the consumption of raw materials and services that are consumed by the process, and the losses, wastes and emissions resulting from the process, paying a particular attention to the flows of chemicals that are being substituted. Ideally inputs should equal outputs, but in practice this is rarely the case, and some judgment is required to determine what level of accuracy is acceptable. The recommended time period to be covered is inputs and outputs over one year (it eliminates seasonal fluctuations).

Inventory of chemicals is needed to identify substances of concern, which shall be substituted. Also, information from the inventory will be needed when performing risk assessment and life cycle assessment (to identify other chemical substances in addition to target substance, which are affected by the substitution).

Input-output analysis will be used when deriving indicator on emissions of target substance. In some cases, e.g. for volatile organic compounds, inputs-outputs at company level will be enough to derive the value of the indicator; in other cases (when emissions occur not only from the production stage, but also during the use phase or disposal) additional information from other life cycle stages will be needed.

Technological processes, inputs-outputs and inventory of chemicals before and after the substitution shall be compared in order to identify changes that will be included and analysed by risk assessment and LCA. They are also a source of initial information for derivation of indicators.

Supporting materials for derivation of indicators are presented:

- emissions of target substances– Chapter 4;
- risk characterisation ratio – Chapter 5;
- environmental impact category indicators – Chapter 6;
- substituted target substances (amounts) – Chapter 4.

4. Emitted and substituted target substances

4.1 General explanation on the emission of substances

The point of departure for evaluating the impacts on environment is related to releases of these chemicals to various compartments: emissions to the air, discharges to surface waters, as well as releases to land and underground. Considerations include emissions of substances during production and releases of these substances during the use phase. The general approach and principles for the environmental exposure assessment correspond to the logic of the safety assessment as laid down in the REACH legislation. Guidance on environmental exposure assessment is elaborated by European Chemicals Agency (ECHA, 2016).

Estimation of emission rates for substances is often accepted as the main challenge in impact assessment. Attempts are made to develop a standardized approach. Environmental release categories (ERC) are designed to describe uses from an environmental perspective (ECHA, 2015) and the default worst case release factors apply. Although, these factors are broadly applicable they often lead to significant over-prediction of releases and, hence, of environmental exposure (Sattler et.al, 2012). Specific environmental release categories (spERCs) are introduced as refined ERC-based emission estimates (CEFIC, 2012; ECHA, 2016). spERCs describe typical operational conditions relevant to the emissions of substances in the environment and define realistic default values of the fractions which are released to various environmental compartments.

spERC factsheets are mainly developed by the chemical industry sectors and trade associations and these organizations are the owners of the spERCs and bears responsibility for the spERC content (CEFIC, 2012). spERCs are made available via industry sector websites. The European Chemicals Industry Association (CEFIC) supports the industry with guidance on how to develop spERCs (CEFIC, 2012). spERCs are in a continuous development and improvement process as facilitated by suggestions from the assessment studies and the feedback from authorities and industry regarding the coverage and completeness of information (Sattler et.al, 2012; Reihlen, 2014).

4.2 Implementation of indicators on emitted and substituted target substances

The LIFE program default tables on assessing environmental impact present default indicators related to the emissions and substitution of chemicals targeted. Time perspective is initial situation (only for emissions), at the end of the project, and 5 years after the completion of the project.

Table 4.1. Example table of default indicators – emissions of target substances.

Chemical	EC no.	Emissions			Units	Environmental and human concerns, environmental compartment affected
		At the beginning	At the end	5 years beyond		
Sodium perborate, perboric acid, sodium salt	239-172-9 234-390-0	37000	0	0	kg/year released	Very high concern for humans and fauna, environmental medium affected- Water

Similarly a table should be prepared for the amount of substituted substances (Table 4.2).

Table 4.2. Example table of default indicators – substitution of target substances

Chemical	EC no.	At the beginning	At the end	5 Years beyond	Units
Di-"isononyl" phthalate	249-079-5	445000	0	0	kg/year

In order to evaluate the impacts of pilot cases implemented in frame of the project, indicators relating to estimated (predicted) changes in releases of hazardous substances and amounts of hazardous substances to be substituted were elaborated for the companies that are project partners. The amounts of substances to be substituted were assessed based on consultations with technical experts in each respective partner company and are straight-forward calculations on how much of the substance that is currently used can be taken out of the production process (all of it or a certain percentage).

The changes in amounts of substances to be released to different environmental compartments are more difficult to assess due to different nature of both the production processes and products involved and the properties of substances addressed. In general, the emissions can be split into two parts: emissions occurring during the production phase and emissions during the use phase of the ready product.

- The emissions from production phase were estimated based on each company's level of knowledge on emissions (or losses) of the target substances during the production phase. If companies did not have respective information, specific environmental release categories (spERCs) were used to model the emitted amounts. The first approach is deemed to be the most accurate one as in this case each company knows their technical processes very well and have made individual calculations about emissions or losses in their specific production process and geographic location. As spERCs are conservative emission models used for generic safety assessments under REACH, the results tend to be higher than those calculated based on individual data.
- The emissions from the use phase of ready products were calculated using spERCs for wide dispersive use in cases when the substances in question remain in the product or in use for a longer time. In cases when the target substances is most likely fully discharged and subsequently reaches the environment (e.g. components in detergents or washing liquids that are being washed away in sewers) use of spERCs was not necessary as all of the used amount of substances were emitted to the environment.

A separate approach was used in case of application of Bisphenol A in canned milk packaging coatings for antibacterial purposes – in this case the producer had concrete information about percentage of cans that are collected back and utilized and cans that are ultimately landfilled. Calculations about amounts of bisphenol A released to the environment were based on this information rather than general approach with use of spERC factsheets and emission multipliers.

In overall, it can be stated that an individual approach was applied to evaluate situation in each partner company, to assess the specific substances and processes involved and information available about them, thus providing the most accurate possible estimation of emissions of hazardous substances to different environmental compartments. In each case the individual approaches and calculations were carefully documented and exact same methodology will be used at the end of the project to ensure that the ex-ante and ex-post results are comparable.

Table 4.3. Use of spERC factsheets for estimation of environmental releases.

Substance	Sector	Use of spERCs fact sheet	Source
DINP	Construction	YES	EFCC spERC factsheet for wide dispersive use of Construction Chemicals
Dibutilyn dilaurate	Construction	YES	EFCC spERC factsheet for wide dispersive use of Construction Chemicals
Sodium perborate	Detergents - soaps	NO*	
Sodium percarbonate	Detergents - soaps	NO*	
Monoethylene glycol	Detergents - soaps	NO*	
Nonylphenol	Construction	YES	EFCC spERC factsheet for the Formulation of Construction Chemicals (mixtures) EFCC spERC factsheet for wide dispersive use of Construction Chemicals
Benzyl alcohol	Construction	YES	EFCC spERC factsheet for the Formulation of Construction Chemicals (mixtures) EFCC spERC factsheet for wide dispersive use of Construction Chemicals
Methylene chloride	Solvents	YES	ESIG spERC factsheet for use in industrial cleaning agents – solvent borne
BPA	Coating of packaging material	NO*	
Propan-2-ol	Solvents in paints	YES	CEPE spERC factsheet for professional spraying - outdoor use - volatiles
Xylene	Solvents in paints	YES	CEPE spERC factsheet for professional spraying - outdoor use - volatiles

*Other methodology was used for calculation

5. Change in chemical risks

5.1 General explanation on the indicator ‘change in chemicals risks’

5.1.1 Aim

The aim of the indicator ‘change in chemicals risks‘ (CCR) is to provide quantitative information on the extent to which the risk of damage to human health (hh) and the environment (env.) has been reduced due to a particular activity or the sum of all relevant project activities. The change of chemical risk is expressed separately for workers, consumers and the environment. The CCR can be developed and compared at the level of an individual product, at company level (e.g. if more than one substance is substituted or one substance in various products) and at project level (overall change of risk achieved by all project activities and contributing institutions).

5.1.2 Understanding

The CCR is an abstract value. It is developed based on hazard and exposure information before and after substitution considering any changes in the use of chemical substances, namely

- on the dose or concentration below which NO damage to human health or animals / the environment is assumed (= safe exposure level) and
- the estimated or measured exposure levels of humans and/or the environment.

The CCR is the difference between the risk characterisation ratios (either for workers, consumers or the environment and for a particular exposure pathway) befor and after substitution. If the value of the CCR is positive, chemicals risks are reduced, if it is negative, chemical risk after substitution are higher than before (this should not occur during the project!). The higher a positive CCR, the higher the reduction of chemical risks. Due to the existence of several CCRs characterising the situation before and after the substitution, a qualitative assessment of the various CCRs is needed.

The CCR is developed from risk characterization ratios (RCRs) for humans and the enviornment which are developed using the model ECETOC TRAM. If a risk is identified (RCR > 1), it may be considered to use a higher tier model to clarify if a risk actually occurs or if it is an artefact, e.g. due to rough assumptions or high safety factors. However, the CCR should be based only on one method, which is ECETOC TRAM.

As the RCR is a measure of RISK and not a measure of actual damage, it does not correspond to everyday experience (workers do not feel intoxicated; fish are still alive in the river). Additionally, damage from chemicals exposure may occur only after a long time. This should be considered in the communication of the CCR / RCR to companies in the project.

If an unacceptable risk is identified from the use of a substance (i.e. using a Tier 2 Model), the need for substitution (or exposure reduction) is obvious. However, there are several reasons, why an RCR could exceed the value of 1 that need to be considered, in particular the use of too rough assumptions, lack of hazard data resulting in high safety factors for the derivation of safe exposure levels or

Also if RCR < 1, substitution may be necessary or recommended because:

- the overall risk from exposure to a substance is not considered in the indicator; there may be other exposure sources of the same substance and the aggregated exposure may be critical;
- the overall exposure levels to (different) substances is increasing; due to cumulative exposures damage may occur even if exposure levels of individual substances are not exceeded or
- just to be cautious, to prevent scandals or strengthen trust in the company / products.

After substitution, the RCR(s) should decrease (CCRs are positive values) indicating an elimination or at least reduction of a negative environmental or health impact as compared to the initial situation (safe(er) in terms of the absence or reduction of risk).

5.1.3 Limitations of the indicator on the change of chemical risks (CCR)

The CCR is derived from the difference between the RCR before and after substitution. Therefore, the limitations of deriving an RCR also apply to the CCR.

An RCR cannot be derived for PBT/vPvB substances and non-threshold CMRs because per definition and, for PBT/vPvBs due to the bioaccumulation potential and persistence, no safe exposure level can be defined.

The derivation of safe exposure levels requires information on the substances' toxicity and eco-toxicity. Where this information is not available, safe exposure levels cannot be easily defined; where only few experimental data are available, the value will include many safety factors and hence overestimate the hazard of a substane. The latter is particularly relevant when comparing two substances with different data availabilities, as the safety factors may be the ONLY reason for the change of risks, potentially indicating an increase of risk due to too conservative safe thresholds. Due to limited resources and capacities, no DNELs will be derived by the project team[5].

In all cases, where a safe exposure level (PNEC or DNEL) cannot be derived, a qualitative assessment on the change of risk will be performed on a case-by-case basis. This means the exposure levels will be determined and compared with the available information on the (eco-) toxicity and/or classification. If this relates to individual components of the mixture, RCRs and changes in chemical risk will be derived and complemented with a discussion on the uncertainties and/or conained substances for which no safe level could be derived.

The derivation of numeric information on the (expected) exposures and the safe exposure levels will be modelled / estimated as no measured data is deemed to be available. Therefore, the exposure levels forming parts of the RCR indicators are more conservative (higher) than the real exposure levels. Hence, unless measured data is available, the RCR will not reflect the actual situation in the company and this needs to be well communicated[6.] With regard to measuring success, this is not relevant

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[5] Deriving safe exposure levels requires toxicological expertise and access to the studies conducted to identify the hazardous effect. This work has not been planned for in the project proposal and respective expertise is not available in the project team. However, in cases where PNEC derivation based on published inforamtion in the ECHA database is possible, it will be implemented to avoid that too much information is lacking for the assessment of substitution impacts.

[6] This may be particularly important in case assessments of workers exposure might indicate a workplace risk which is overestimated by the models.

because the same methodology underlies the assessments for each of the cases, and the related uncertainties should be the same for all indicators.

A CCR for the air is developed using a non-standard method based on a model for air dispersion from Estonia and using the DNEL for consumers (inhalation).

5.1.4 Justification and evaluation

The chemical risk is the central measure driving chemicals risk management and indicating the need and urgency for action. Therefore, it is reasonable to select the change in the chemical risks for humans, differentiated into workers and consumers and the environment that is achieved by the implementation of a substitution. This is particularly true, as the currently used methods for the assessment of lifecycle impacts does not reflect the risks for workers and consumers (to a sufficient extent). In general, a positive CCR indicates a reduction of chemical risk, i.e. an improvement of the environmental or health situation whereas a negative CCR indicates a worsening of the situation.

The use of the CCR as one indicator to measure substitution success could raise awareness on chemical safety assessment and bring a new perspective to the company policy and any indicators already in place.

The CCRs from raw materials production and from the waste stage are not considered in this concept. Although this information may influence the overall assessment of changes in risk, the borderlines for measuring project impacts will only include those aspects, which are under the direct influence of the companies. In addition, the CCRs from the manufacturing of input substances are not considered in this concept, mainly for two reasons:

- they relate to different substances than the substance that shall be replaced and its alternative (they are input material to the production of the hazardous substance / its alternative), and
- the efforts to collect information are regarded as disproportionate to the level of information that would be obtained, because substance manufacture usually does not give rise to high emissions and hence, low RCRs/CCRs are expected which are not likely to be meaningful.

The RCRs/CCRs of the waste stage are not included also because of a lack of methods to model emissions from waste treatment processes.

The CCRs are derived separately for workers, consumers and the environment and for different pathways (c.f. details below) which are regarded as the most relevant and feasible (in particular with regard to the availability of data and methods) in order to identify the changes in chemical risks. An aggregation to a “Total change of risk” for workers and consumers will be developed if useful to communicate or present the change in risks. The CCRs cannot be further aggregated (e.g. summing up changes of risks to “humans”).

Whether or not a shift of risk is an improvement or not is a case-by-case decision, taking the extent of the new risk into account.[7]

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[7] This will be decided on and implemented flexibly by the project team and decisions will be transparently documented.

5.1.5 Overview of RCRs as a basis to derive CCRs

5.1.5.1 Quantification of the RCR

In accordance with the EU methodology for regulatory chemicals risk assessment, e.g. under REACH or the Biocides Regulation, a chemical risk is quantitatively expressed as the ratio between an exposure level and the concentration / dose of a substance below which no damage is expected.

Equ. 1: RCR for the aquatic environment = PEC / PNEC

Equ. 2: RCR for humans = Exposure level / DNEL

PEC = predicted environmental concentration = a quantitative value for the concentration of a substance in the environment derived from the amount emitted in relation to the use assessed and its fate and behaviour in the environment.

PNEC = predicted no effect concentration = concentration of a chemical below which no adverse effects on organisms / the environment are expected. The value is derived from information on a substance's hazards derived from testing or other methods.

DNEL = derived no effect level = dose or concentration of a substance below which no adverse effects on human health are expected. Different values are defined for acute and chronic toxicities and the three pathways inhalation, ingestion and skin contact as well as for workers and consumers.

In addition and where relevant, we will assess the risks from air emissions to human health (via the environment) using

Equ. 3: RCR for the air compartment = PEC / $DNEL_{cons,chronic,inhalt}$

5.1.5.2 PBTs/vPvBs and non-threshold CMRs

For PBTs/vPvBs no RCR can be determined. If a substitution concerns a PBT/vPvB the emission level of the substance is used as an indicator (Section 4 on emitted amounts) and a qualitative discussion on the overall change of chemical risks will be developed.

For non-threshold CMRs under REACH so called DMELs (derived maximum exposure levels) may be derived and published by REACH registrants. The DMEL anticipates that a certain likelihood of cancer deaths is acceptable. Therefore, the DMEL cannot be compared to a DNEL and does not serve as appropriate value to compare RCRs for different substances. Therefore, for non-threshold CMRs, the exposure level[8] as such is used as risk indicator and a qualitative discussion on the overall change of chemical risks will be developed.

5.1.5.3 Dermal contact

A quantitative assessment of dermal risks is frequently not possible because no quantitative DNELs are available. If this is the case, the exposure level can nevertheless be derived and can be used as an indicator.

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[8] In this case, the exposure level is used as this integrates the mobility of a substance. If a CMR that is highly volatile were replaced by one, which is not volatile, this would already be an improvement for workers and therefore, the exposure level is a more relevant indicator than the emitted amount.

5.1.5.4 Differentiation of RCRs/CCRs

For the purpose of measureing the impact of substitution on the chemical risk from the use of substances and mixtures in products and processes the following RCRs and CCRs are developed as a default.

For workers

- Long-term inhalation, long-term dermal,
- Short-term inhalation, short-term dermal

For consumers

- Inhalation, ingestion and dermal

For the environment

- STP
- local freshwater
- local freshwater sediment
- man via the environment

Which types of RCRs/CCRs are relevant to a particular case and can be developed depends on the substance hazards (i.e. if an effect threshold exists), the availability of hazard data and the relevance of the exposure pathways of the relevant substances.

For example, no RCR/CCR for dermal toxicity needs to be derived if none of the substance(s) involved in the substitution causes harm to the skin. However, if any of the substances causes skin effects, the RCRs/CCRs needs to be derived and for sustances without skin effects, the RCR is defined as “0” to represent absence of a respective risk.

A substance, which is only used in industrial processes would not cause any consumer exposure; hence no RCRs/CCRs for consumers are relevant.

5.1.5.5 Scope and interpretation of overall RCRs/CCRs

In order to determine the change of chemical risk all changes are considered that affect substances that are classified either for the environment or for human health and which are included in the mixtures under assessment in concentrations above the limits for identification in the safety data sheet, unless another decisions is made by the project team.[9] This means if the substitution of a substance requires the use of two or more substances, the overall change of chemical risk needs to take into account both of the substances used instead. If a mixture is substituted by another mixture, the risk reduction results from the changes of chemical risk for all relevant components (i.e. classified and contained above specified concentration thresholds) in the mixture. The scope of the indicators must therefore be determined / assured when the full extent of the substitution is known.

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[9] Classification due to physical-chemical hazards is not rearded relevant (no toxicity/eco-toxicity). The assessment is limited to substances above concentration thresholds for identification in the safety data sheet in order to avoid limitations in data availability and/or confidentiality concerns.

To determine the overall change of the chemical risk, the values of the RCRs within the same category (e.g. workers, long-term inhalation or consumers, oral) are added up for all relevant substances.

Equ. 4: $RCR_{\text{local, freshwater}} = \sum RCR_{\text{local, freshwater,n}}$

The RCRs for all relevant substances used before the substitution are compared to the RCRs of all relevant substances used after the substitution to determine the CCR. Substances for which the use (including the amount!) is the same before and after the substitution are not included in the calculation, because there are also no changes in RCRs.

Equ. 5: $CCR = \sum RCR_{\text{before substitution}} - \sum RCR_{\text{after substitution}}$

If the use of a substance is not substituted but the use amount is changd the risk characterisation ratio and hence the CCR are changed, too. Whereas the safe exposure level would remain unchanged, the (expected) exposure level would decrease. Hence, this type of change must be considered, too. The Examples of how to interpret the CCRs are shown in the following table.

Table 5.1. Examples of how to develop and interpret CCRs

RCR of substance A (to be substituted)	RCR of substance B (alternative)	CCR	Result
Workers, inhalation, long-term	No respective hazard → RCR = 0	$RCR_A - 0 = RCR_A$	Positive → risk has been reduced by 100%
No respective hazard → RCR = 0	Workers, inhalation, short-term	$0 - RCR_B = -RCR_B$	Negative → risk increased
Water, local = 0.2	Water, local = 0.1	$RCR_A - RCR_B = 0.1$	Positive → risk reduction by (50%)

5.1.5.6 Application of CCR indicators

The CCRs may be used to give feedback on the impacts of substitution to the companies (work packages B1 and B2).

For activity B1 (substitution cases already outlined in the project proposal) all relevant CCRs should be developed, taking into account the type of products and processes and related exposures of humans and the environment. Hence, when the scope and extent of substitution are clarified, including which substances will be used to replace a substance and which changes in composition of the product or the use of chemicals is related to this, the relevant indicators should be determined and developed for the situation before and after the substitution.

For the “light cases” (B2) a similar approach is intended but may have to be adapted case-by-case, depending on the actual changes they aim to implement (which may not be a substitution at all). Which of the CCRs are the most relevant for those cases will be decided by the project team, if related information is available.

To quantify the overall change in chemical risk due to the project activities, the CCRs of the the individual activities will be presented and, where possible and useful be summed up. In addition, a qualitative discussion on the meaning and limitations of the CCRs will be developed and a graphical presentation will be developed. Table 5.2 lists the CCRs that are aimed to be developed to show the project impacts on chemicals risks.

Table 5.2. Overview of CCRs to show risk reduction for workers, consumers and the environment

Workers	Consumers	Environment
Long-term inhalation	Inhalation	Local, freshwater
Long-term dermal	Dermal	Local, freshwater, sediment
Short-term inhalation	Oral	STP
Short-term dermal		Man via environment

5.2 Guidance for indicator derivation

The steps and tools for the indicators development is are shown in the following figure. Some detailed information on the individual steps are provided in the following sections.

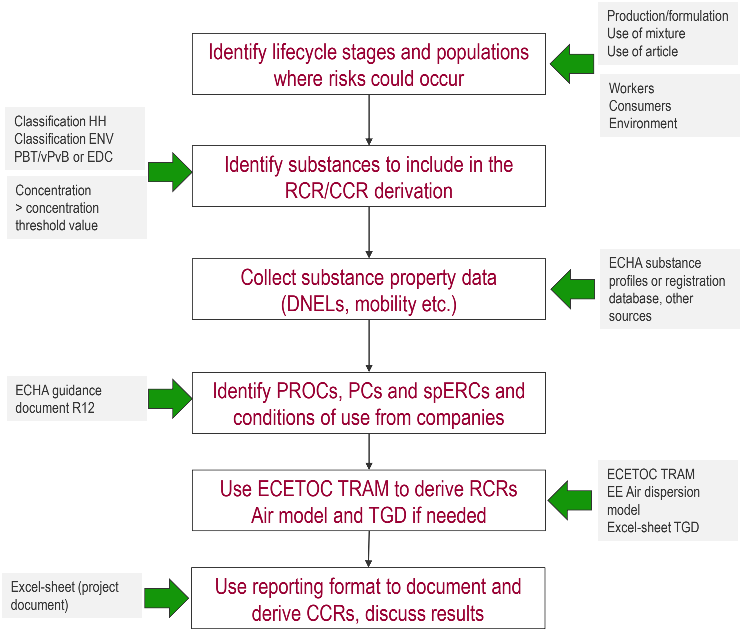


Fig. 5-1: Steps and tools to develop the CCRs

5.2.1 Identification of relevant exposure patterns

The following table links the lifecycle stages with the exposed population and the types of DNELs/PNECs that should be collected from ECHAs information sources.

Table 5.3. Relation between lifecycle stage, exposed group, exoposure durations and exposure pathways (human health)

	Exposed humans	**Exposure duration**	**Possible pathway**
Formulation and/or use of mixture in installations or by professional users; this includes the use of mixtures for the production of articles	Workers	Short-term	Inhalation
			Dermal
		Long-term	Inhalation
			Dermal
Use of a substance / mixture by consumers	Consumers	Long-term	Inhalation
			Dermal
			Oral
Service life of an article	Consumers	Long-term	Inhalation
			Dermal
			Oral

The selection of the specific DNELs is limited in most cases by the data availability. Where DNELs exist in the ECHA database, these should be used.

Table 5.4 provides similar information for the environment but details only those environmental compartments, for which RCRs should be derived. For VOCs the derivation of RCRs for air should be considered, while this is not useful for non-VOC substances.

Table 5.4. Relation between use pattern and exposures of the compartments, for which an RCR should be derived.

	Emission to	Scale	Compartments
Formulation and/or use of a mixture in industrial installations, including for the production of articles	Water	Local	Freshwater, local
			Freshwater, sediment
			STP
			Man via environment
Use of a substance / mixture by consumers or professional users	Water, Air, Soil	Regional	Freshwater, local
			Freshwater sediment
			STP

	Emission to	Scale	Compartments
			Man via environment
Service life of an article	Water, Air, Soil	Regional	Freshwater, local
			Freshwater sediment
			STP
			Man via environment

5.2.2 Identification of relevant substances

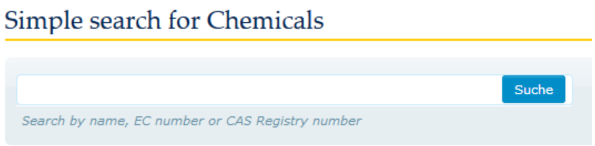
Only substances as such or included in mixtures, which fulfil the following conditions are considered in the indicator development and therefore only for those it is necessary to collect information and derive RCRs/CCRs

- The substances is classified for human health or the environment or it is a PBT/vPvB or an endocrine disruptor
- It is used as such or included in a mixture above the concentration limits
- The amount of the substance as such or in the mixture is reduced (up to zero) due to the substitution

If there are classified substances or PBT/vPvBs or EDCs in a mixture below the concentration thresholds for identification in the safety data sheet, it may be decided on a case-by-case basis that this is considered relevant and therefore included in the derivation of CCRs.

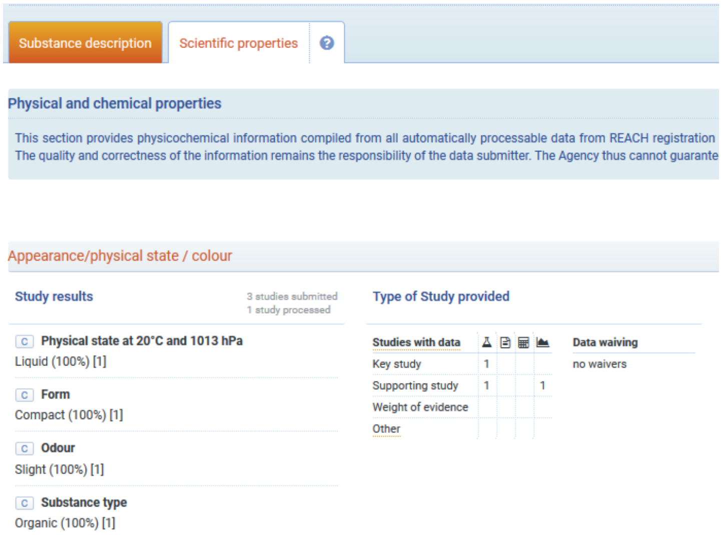
5.2.3 Obtaining safe exposure levels (DNELs, PNECs)

The safe exposure levels of a substance should be identified from ECHA's databases. The easiest option it to search for the brief profile of the relevant substances and extract the available DNELs/PNECs from it (c.f. tab on 'scientific properties'). The substance can be searched for by name, CAS-number or EC-number.


Simple search for Chemicals

Search by name, EC number or CAS Registry number

Fig. 5.1. ECHA's search form



Physical and chemical properties

This section provides physicochemical information compiled from all automatically processable data from REACH registration
The quality and correctness of the information remains the responsibility of the data submitter. The Agency thus cannot guarante

Appearance/physical state / colour

Study results 3 studies submitted
1 study processed

C **Physical state at 20°C and 1013 hPa**
Liquid (100%) [1]

C **Form**
Compact (100%) [1]

C **Odour**
Slight (100%) [1]

C **Substance type**
Organic (100%) [1]

Type of Study provided

Studies with data	⚗	📄	🖩	📈
Key study	1			
Supporting study	1			1
Weight of evidence				
Other				

Data waiving
no waivers

Fig. 5.2. Brief profile

In the brief profile, physical-chemical information as well as available DNELs and PNECs are provided. If no information is presented, it should be checked if additional information is available in the registration file that can be obtained by searching the registration database. The information should be used from the joint registration (symbolised by several persons) in the third last column.


Showing 45 results.

Name	EC / List no.	CAS no.	Registration type	Submission type	Total tonnage band	
Formaldehyde	200-001-8	50-00-0	Intermediate	👤	Intermediate Use Only	⊙
Formaldehyde	200-001-8	50-00-0	Full	👥	1 000 000+ tonnes per annum	⊙
Formaldehyde, oligomeric reaction products with 1-chloro-2,3-epoxypropane and phenol IUPAC name: Formaldehyde	500-006-8	9003-36-5	Full	👥	10 000 - 100 000 tonnes per annum	⊙

Fig. 5.3. Selection of relevant files from the search results

5.2.4 Options in case DNELs/PNECs are missing

If no DNELs / PNECs are available from ECHA's database this may have different reasons, among others:

- No data are available, e.g. as the substance is registered in a lower tonnage band
  In this case, further action is necessary.
- Data are available but they indicate that there are no effects; i.e. a DNEL does not have to be derived for systemic inhalation exposure.
  In this case, the RCR can be defined as "0" due to lack of hazard.

- The registrant does not need the value for his risk assessment, as no respective exposures occur
  In this case, data may be available but it was not used to derive a DNEL.

If no DNELs are published in ECHA's data base or other information sources, no RCR will be developed.

If no PNECs are published but data are available from ecotoxicity testing, the PNEC will be derived according to the rules set out in ECHA's guidance document R16.

Alternative values, such as EQS or OELs are not used to derive RCRs because the methodologies differ and the RCR would not be comparable.

The databases upon which DNELs/PNECs are derived in ECHA's database is documented in the project reporting file for the CCR derivation, as the number and type of studies influence the scale of the safety factors applied in the derivation of DNELs/PNECs by the registrants. Hence, inconsistencies in RCRs/CCRs that may be due to differences in the availability of information can thereby identified and discussed.

If no safe exposure levels (DNELs/PNECs) for individual substances in a mixture are available (regardless of whether for the chemical that should be substituted or its alternative), the CCRs are developed for the remaining substances. The influence of the substance(s) without DNELs/PNECs on the change of chemicals risks is approximated qualitatively using the exposure levels and any available information on the toxicity/ecotoxicity in the indicator report. This will be done on a case-by-case basis.

If substances are not registered, it is likely than no DNELs or PNECs are available. Hence, a qualitative assessment of the impact on the change of risk from those substance has to be done based on the exposure levels and any hazard information that can be obtained from other information sources than ECHA's databases.

5.2.4 Obtaining exposure levels

The tool for deriving exposure levels and RCRs for humans and the environment is ECETOC TRAM. It allows processing several substances together (e.g. if contained in a mixture), has a comparatively simple input form and provides RCRs in accordance to the above listed parameters. If all teams use the same tool, information is comparable and problems in indicator derivation can be more easily discussed and resolved.

If data from the companies are available on the exposure levels, e.g. for workers, this information may be used to derive RCRs, too. However, in this case the same data needs to be used for the substance/mixture to be substituted and the alternative used after substitution took place.

ECETOC TRAM

ECETOC TRAM includes all default values necessary to RCRs for workers, consumers and the environment, at least at a lower tier level. The tool is available for free and is comparatively easy to use. A manual is available for the users. RCRs are calculated which could directly be used as indicator in the project.

For the workers RCRs, the DNELs need to be included and the PROCs be selected, which cover all production steps that the substance is used in. Guidance on what a PROC means is provided in ECHA's guidance document on worker exposure. In addition, the time a worker handles the substance and the risk management measures available should be specified. The tool calculates the exposure levels automatically.

For consumers RCRs, the DNELs for consumers should be inserted and the product category. The assessment is possible only for the use of mixtures but no models are available to assess exposure from articles in ECETOC TRAM. For this, if this option is chosen, a different tool must be used (c.f. below).

The environmental module of ECETOC TRAM allows calculating all RCRS that are identified as relevant. However, also here the service life cannot be assessed, because the calculations only function, if a spERC or ERC are entered (and there is none for the service life of articles). A different option must be used for this (c.f. below).

5.2.5 Higher tier assessments (not for indicator development)

Stoffenmanager

A useful model, which could be used to refine a tier 1 risk assessment for workers by ECETOC TRAM is the Stoffenmanager (www.stoffenmanager.nl), for which a free version is available on the internet to model exposure levels via inhalation and derive risk levels for dermal exposure. The substance(s) for which the exposure or risk should be modelled needs to be entered and the workers' activities as well as the conditions the workplace be specified. For the inhalation exposure the programme automatically calculates a "task concentration" – corresponding to a short term exposure and a "daily average concentration" – corresponding to a long-term exposure. For dermal risk the programme derives a risk level and differentiates into high, medium or low risk.

ConsExpo and emission tool

The most frequently used tier 2 model allowing estimation of consumer exposures to mixtures is ConsExpo. The web tool includes options to assess emissions from articles.

spERCs and TGD excel-sheet

It is possible that some spERCs exist but are not integrated in ECETOC TRAM. If this is the case, the emitted amount must be calculated separately and the PEC be modelled using the Excel-Spreadsheet of the EU TGD by RIVM (c.f. below). The list of available spERCs is provided in the following table (first check, if they are integrated in ECETOC TRAM).

Table 5.5. Links to spERCs on the associations' websites

Sector group	Coverage	Link
ACEA	Use of coatings in automotive industry	http://www.acea.be/publications/article/reach-extended-safety-data-sheets
A.I.S.E.	Manufacturing and using detergents, maintenance products, industrial cleaners and	http://www.aise.eu/our-activities/product-safety-and-innovation/reach/environmental-exposure-assessment.aspx

Sector group	Coverage	Link
	metal treatment products	
ATIEL	Manufacturing and using of lubricants / lubricant additives	http://www.atiel.org/reach/suppliers/11-public-content/reach-content/68-spercs
CEPE	Manufacturing and using coatings, inks, artist colours	http://www.cepe.org/efede/public.htm#SPERCs_appl
Cosmetics Europe	Manufacturing and using body care products, cosmetics	https://www.cosmeticseurope.eu/safety-and-science-cosmetics-europe/reach-and-chemicals/use-and-exposure-information.html
ECMA	Manufacturing catalysts	http://www.cefic.org/Documents/Industry%20sectors/ECMA/ECMA%20-%20SPERC%20Factsheet%20-%20Manufacture%20of%20Metal-containining%20Catalysts%20V5%2027Feb%202012.pdf
ECPA	Crop protection products	http://www.ecpa.eu/information-page/regulatory-affairs/reach
EFCC	Construction chemicals	http://bauchemie.vci.de/wiki/SPERC_UseR_CC
ESIG	Manufacturing and using solvent and solvent-based products	http://www.esig.org/en/regulatory-information/reach/ges-library/ges-spercs-2
ETRMA	Manufacturing rubber products	http://www.etrma.org/activities/chemicals/reach/emission-factors
EURO-METAUX	Manufacturing and using metals	http://www.arche-consulting.be/Metal-CSA-toolbox/spercs-tool-for-metals
FEICA	Manufacturing and using adhesives and sealants	http://www.feica.eu/ehs-sustainability/reach/feica-use-descriptors
IFRA	Manufacturing, compounding fragrance materials.	http://www.ifraorg.org/view_document.aspx?docId=23068

The emitted amount is calculated by multiplying the daily use amount with the release factors indicated in the spERC. The daily use amount is obtained from the annual use amount divided by the number of working days at which the substance is used.

The PEC can then be calculated by inserting the emitted amounts into the TGD excel-spreadsheet.[10]

Environment, air

To derive the RCR for air, a PNEC air is needed, which is not normally available due to a lack of (requirements to generate) data on environmental toxicity via air. Therefore, in this project, the DNEL for consumer inhalation is used as “surrogate PNEC_{air}” for humans in a close distance to any point sources / industrial installations.

Emissions to air are only calculated for industrial installations, because a) no effects are likely to occur from professional / consumer uses due to low amounts emitted and high dilution volumes (very low environmental concentrations) and b) exposures from articles are reflected in the human health assessment already.

For VOC / solvents used at industrial sites as processing aids the releases may be assumed with 100%. For substances which are not used as processing aids but may be emitted from the process, either company information can be used (e.g. measured in waste gases and the waste gas volumes) or estimated using spERCs (c.f. above). To determine the environmental concentration at which human neighbours could be exposed to these substances, a calculation for air dispersion according to Estonian legislation can be used[11].

The following information is needed (from the companies) to use the model and calculate the environmental concentration at 100 m from the emission source:

Table 5.6.

Input data			Unit	Explanation
1	Sedimentation coefficient			Gas and aerosols from combustion = 1; other aerosols = 2, coarse particles = 3
2	Height of emission source from ground		m	chimney height
3	Temperature of waste gas		°C	actual temperature minus 20; if temperature is below 30: enter 10
4	Diameter of emission source		m	diameter of chimney

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[10] Information on which information needs to be includedc in the excel-file is inlcuded in the project CCR reporting format.

[11] An excel file including the calculation is provided separately.

Input data			Unit	Explanation
5	Air volume extracted	🟨	m3/h	extraction of waste gase by treatment device
6	Substance amount emitted per day	🟧	kg/d	information to calculate massflow, can be omitted if emission concentration is known
7	Operating hours per day	🟧	h/d	information to calculate mass flow; can be omitted if emission concentration is known
8	Mass flow of substance	▨	g/s	calculated from 7 and 8, if known, can be entered directly
Result	**Concentration at 100 m from source**	🟩	**µg/m3**	**To be compared with DNEL consumer chronic**

The resulting value (concentration at 100 m from source) should be compared to the DNEL for the inhalation route (chronic) for consumers. If the quotient of the environmental concentration and the DNEL exceeds 1, a risk exists.

5.3 Developing CCRs

The CCRs are developed by substracting the sum of all risk characterisation ratios for each of the different populations and exposure pathways and subtracting the value after substitution from that before substitution. The following CCRs could be available, if all indicators can be developed:

- CCR workers,inhalation
    - long-term
    - short-term
- CCR workers,dermal
    - long-term
    - short-term
- CCR consumers inhalation
- CCRconsumers dermal
- CCR consumers oral
- CCRenvironment
    - STP
    - freshwater local
    - freshwater sediment
    - man via env

The calculation of the sums of RCRs and the CCRs are facilitated by the project reporting format (excel-file). For each indicator, a qualitative discussion has to be developed presenting all information relevant for its interpretation, including if no PNECs or DNELs could be used.

6. Life cycle impact (LCA) indicators

6.1 General explanation on the LCT and LCA

Life Cycle Thinking (LCT) is a core concept in Sustainable Consumption and Production (SCP) for business and policy. **The environmental pillar of LCT is supported by Life Cycle Assessment (LCA)**, an internationally standardised tool (ISO14040 and ISO14044) for **the integrated environmental assessment of products** (goods and services). Upstream and downstream consequences of decisions must be taken into account to help avoid the shifting of burdens from one impact category to another, from one country to another, or from one life cycle stage to another. **LCA is a methodological tool used to quantitatively analyse the life cycle of products/activities within the context of environmental impact.**

As the full Life Cycle Assessment requires a lot of input data and calculations, a **simplified** LCA approach will be applied in the project. Looking at the industrial sector, taking LCA as an approach means going beyond the narrower traditional focus on an enterprise's production facility.

The Life Cycle Assessment consists of four phases (ISO 14040):

1) In the *Goal and scope definition phase*, the aim of the LCA is defined and the central assumptions and system boundaries choices in the assessment are described.
2) In the *Life Cycle Inventory (LCI) phase*, the emissions and resources are quantified for the chosen products in scope of the chosen system boundaries.
3) In the *Life Cycle Impact Assessment (LCIA) phase*, these emissions and resource data are translated into indicators that reflect environment and health pressures as well as resource scarcity. This calculation is based on factors which represent the predicted contribution to an impact per unit emission or resource consumption. These factors are generally calculated using already elaborated scientific models.
4) In each phase, in the *Interpretation phase*, the outcome is interpreted in accordance with the aim defined in the goal and scope of the study.

LCA framework from ISO 14044 (Fig. 6.1):

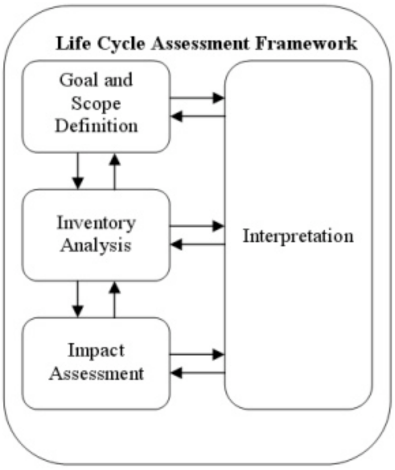


Fig. 6.1. LCA Framework (ISO 14044)

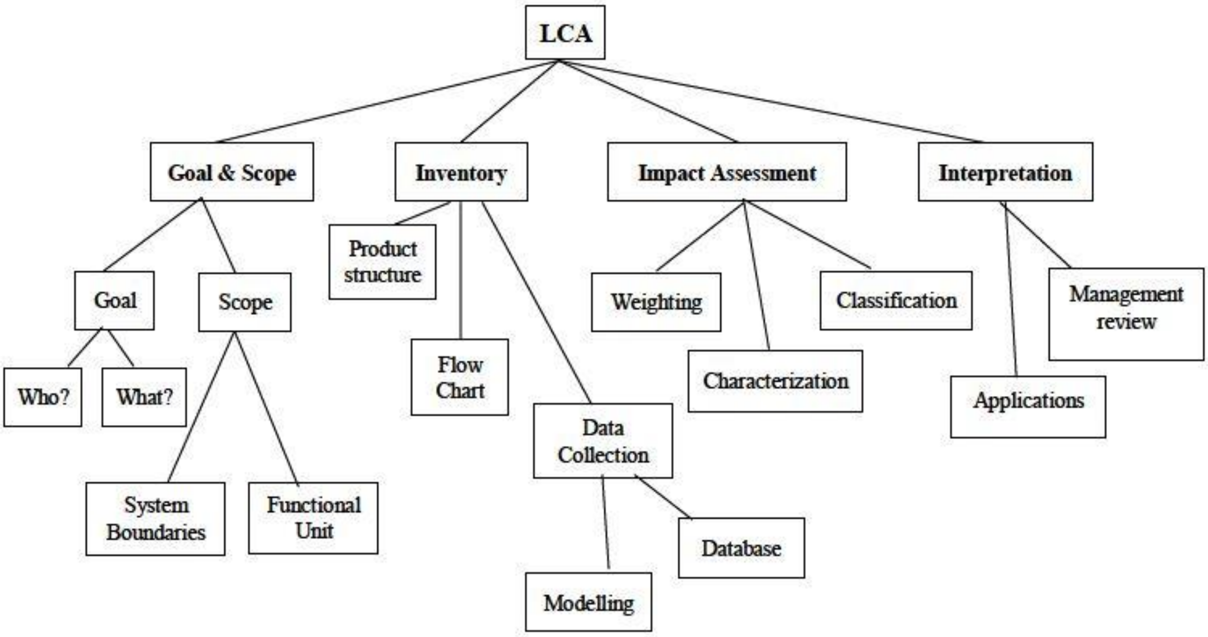


Fig. 6.2. Logical structure of LCA based on 14001 and 14004 (Weighting step includes normalization)

A number of methods used for Life cycle impact assessment (LCIA) **convert the emissions of hazardous substances and extractions of natural resources into impact category indicators at the midpoint level** (such as acidification, climate change, ecotoxicity and etc.), while others employ impact category indicators at the **endpoint level** (such as damage to human health and damage to ecosystem quality).

6.1.1 Aim

The aim of the LCA indicators is to provide quantitative information on the extent to which the negative impact to environment, human health and resources have been reduced due to the substitution of hazardous chemicals during project activities. Impact can be reduced for three areas of protection (AoP): environment, human health and resources.

6.1.2 Understanding

The method applied in the project for deriving LCA indicators is called ReCiPe (ReCiPe 2008). Like many other methodologies on LCA it **provides a recipe to calculate life cycle impact category indicators**.

LCA compared with the simplified LCA differs in its scope, depending on the assessor's **needs and resources**. A full LCA would require all processes to be included from the extraction processes of raw materials to the recovery and disposal of the product, hence great amount of resources of time and money required. On the other hand, in simplified LCA, the assessor may ignore the processes that he/she thinks has a negligible impact. The comprehensiveness of a LCA is defined by the scope of its system boundaries (which processes of life cycle are included) and the selection of impact categories.

A case specific inventory for the examined process is used, complemented by industry average data for the rest of the life cycle (http://www.eebguide.eu/?p=922). The primary objective of the ReCiPe method, is to transform the long list of Life Cycle Inventory results, into a limited number of indicator scores (characterisation). These indicator scores express the relative severity on an environmental impact category. In ReCiPe we determine indicators at two levels:

- Eighteen midpoint indicators
- Three endpoint indicators

Justification for methodology

There are several LCIA methodologies apply essentially the same principles or minor variations for given impact categories. ReCiPe is a follow up of Eco-indicator 99 and CML 2002 methods. It integrates and harmonises midpoint and endpoint approach in a consistent framework. Although initially integration of the methods was intended, most important impact categories have been redeveloped and updated. As regard to chemical substances - approximately 3000 chemical substances are covered and eighteen impact categories are addressed at the midpoint level:

1) climate change (CC)
2) ozone depletion (OD)
3) terrestrial acidification (TA)
4) freshwater eutrophication (FE)
5) marine eutrophication (ME)
6) human toxicity (HT)
7) photochemical oxidant formation (POF)
8) particulate matter formation (PMF)
9) terrestrial ecotoxicity (TET)
10) freshwater ecotoxicity (FET)
11) marine ecotoxicity (MET)
12) ionising radiation (IR)
13) agricultural land occupation (ALO)
14) urban land occupation (ULO)
15) natural land transformation (NLT)
16) water depletion (WD)
17) mineral resource depletion (MRD)
18) fossil fuel depletion (FD)

Midpoint indicators in ReCiPe method

Ozone depletion: The characterization factor for ozone layer depletion accounts for the destruction of the stratospheric ozone layer by anthropogenic emissions of ozone depleting substances (ODS). The unit is yr/kg CFC-11 equivalents.

Human toxicity and ecotoxicity: The characterization factor of human toxicity and ecotoxicity accounts for the environmental persistence (fate) and accumulation in the human food chain (exposure), and toxicity (effect) of a chemical. The unit is yr/kg 1,4- dichlorobenzeen (14DCB). USES-LCA 2.0 calculates compartment-specific fate factors for 1 freshwater, 1 sea, 3 oceanic and 7 soil compartments. Emission compartments identified were urban air, rural air, freshwater, seawater, agricultural soil and industrial soil on the Western European scale. The nested multimedia fate model Simplebox 3.0, developed by Den Hollander et al. (2004) and included in the newest version of EUSES (EC, 2004), forms the basis of the update of USES-LCA. Worker and consumer exposure is not included in simplified LCA (Nor in full LCA).

Radiation: The characterization factor of ionizing radiation accounts for the level of exposure. The unit is yr/kg Uranium 235 equivalents.

Photochemical oxidant formation: The characterization factor of photochemical oxidant formation is defined as the marginal change in the 24h-average European concentration of ozone (dCO3 in kg·m^3) due to a marginal change in emission of substance x (dMx in kg·year^{-1}). The unit is yr/kg NMVOC.

Particulate matter formation: The characterization factor of particulate matter formation is the intake fraction of PM_{10}. The unit is yr/kg PM_{10} equivalents.

Climate change: The characterization factor of climate change is the global warming potential. The unit is yr/kg CO_2 equivalents.

Agricultural and urban land occupation: The amount of either agricultural land or urban land occupied for a certain time. The unit is m^2 *yr.

Natural land transformation: The amount of natural land transformed and occupied for a certain time. The unit is m^2 *yr.

Marine eutrophication: The characterization factor of marine eutrophication accounts for the environmental persistence (fate) of the emission of N containing nutrients. The unit is yr/kg N to freshwater equivalents.

Freshwater eutrophication: The characterization factor of freshwater eutrophication accounts for the environmental persistence (fate) of the emission of P containing nutrients. The unit is yr/kg P to freshwater equivalents.

Fossil fuel depletion: The characterization factor of fossil depletion is the amount of extracted fossil fuel, based on the lower heating value. The unit is kg oil equivalent (1 kg of oil equivalent has a lower heating value of 42 MJ).

Minerals depletion: The characterization factor for minerals depletion is the decrease in grade. The unit is kg Iron (Fe) equivalents.

Freshwater depletion: The factor for the freshwater depletion is the amount of fresh water consumption. The unit is m^3.

Please visit http://www.leidenuniv.nl/cml/ssp/publications/recipe_characterisation.pdf for the detailed description of each impact category and methods. Impacts to the environment, resources and human health are usually evaluated by the following scheme (Fig. 6.3).

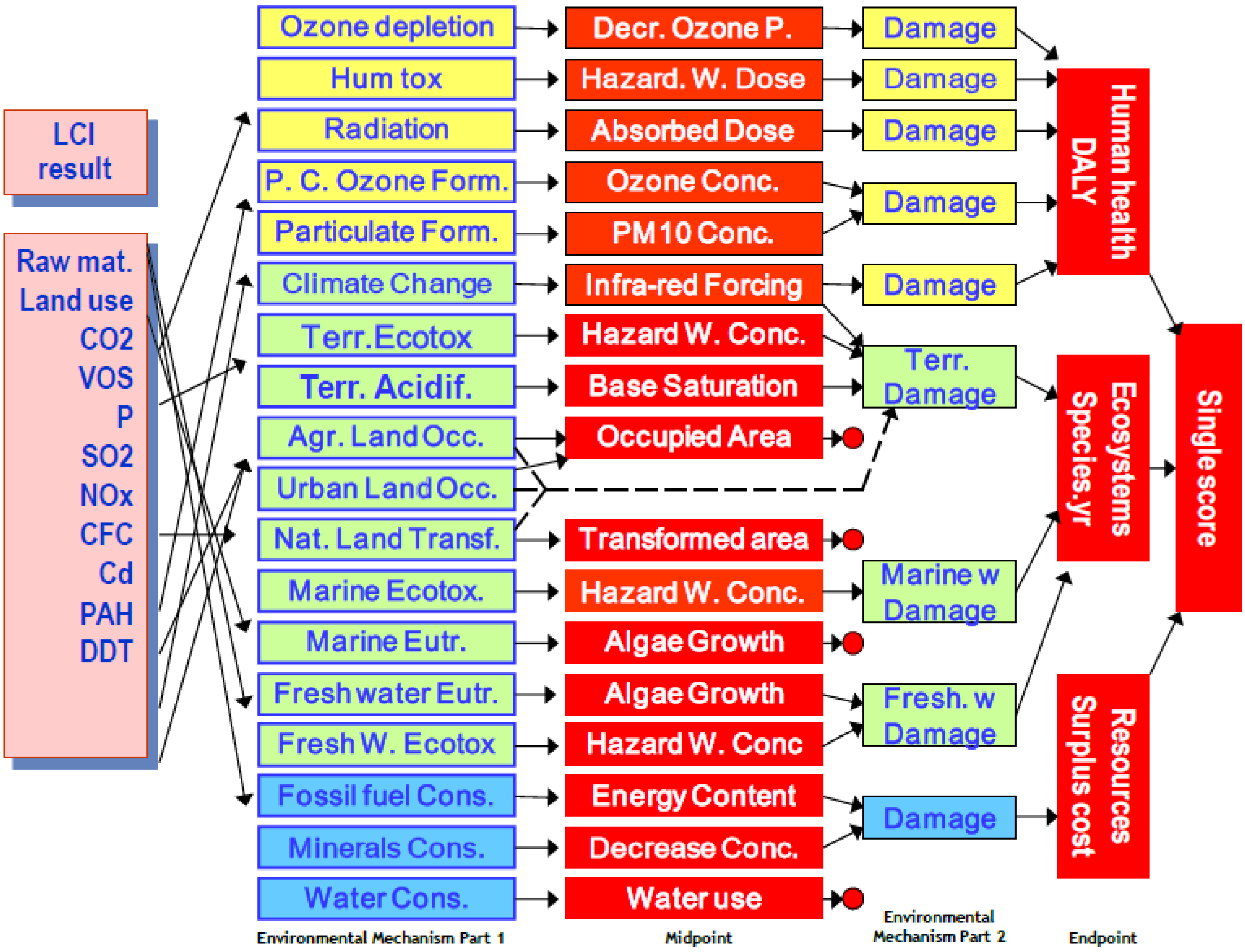


Fig. 6.3. Common LCA methodology connecting LCI to impact indicators (ReCiPe 2008, May 2013)

The characterization factors for each of the above mentioned impact categories can be used to compare the initial and final situation within each impact category itself. To be able to compare the severity of the impact between impact categories, a normalisation step should be implemented. Normalisation is done by normalising the environmental impact of the product to the environmental impact of the average EU citizen, for each impact category.

6.1.3 Limitations

- The scope of LCI is not easy to justify, and missing information from companies, processes are usually a common case. Although, it is possible to use industry average values as complementary to prepare a LCI.
- Assumptions should be made where there is missing information.
- Allocation of impacts among products can be problematic if there is more than one product is produced during a process.
- Definition of functional unit is clear only if the products serve the same quantifiable function.
- Workers and consumer safety is not included.

6.1.4 Justification and evaluation

Environmental policies on substances have so far been formulated mainly to reduce emissions of hazardous substances. The substitution as such is replacement of a chemical substance/process by another chemical substance/process which has a similar function but which is less harmful to the environment and to human health. But mapping out a path towards a more sustainable society requires detailed information on the environmental consequences of proposed activities and changes. Therefore, LCA with its aim of comprehensively identifying all relevant impacts from products and processes is a valuable tool for this project, builds up on the emission / release indicators and complements the risk indicators.

6.1.5. Overview of Scope and Inventory Analysis of LCA

Scope: The scope of the LCI should be defined at the beginning of the assessment. After the initial inventory analyses the scope might need to be updated. Scope must be defined for the system boundaries (which life cycle stages will be included in the assessment), for the LCI to be gathered (for which processes direct quantitative data will be gathered) and for the impact categories to be assessed. For Simplified LCA as will be used in this project, there is no reason to define the scope from cradle to grave for the product.

For the indicator derivation in this project, the entire lifecycle of the substance that should be substituted will be assessed. This scope is also applied to any alternative used.

Generally, applying the LCA, the impacts should be identified for a defined entity of the product which does a predefined function (e.g. for a paint, covering 1 m^2 wall for a year). This is called the ‘functional unit’.

The functional unit will be defined individually for each substitution case.

Inventory Analysis: LCI for Simplified LCA can be formed by using only the input-output analysis data from the company, including direct emissions. In this project, it is considered we would be able to have information on use phase as well (i.e. inputs/outputs during use phase). The information on the disposal phase considered to be out of reach, but might be used if readily available (Fig. 6.4.).

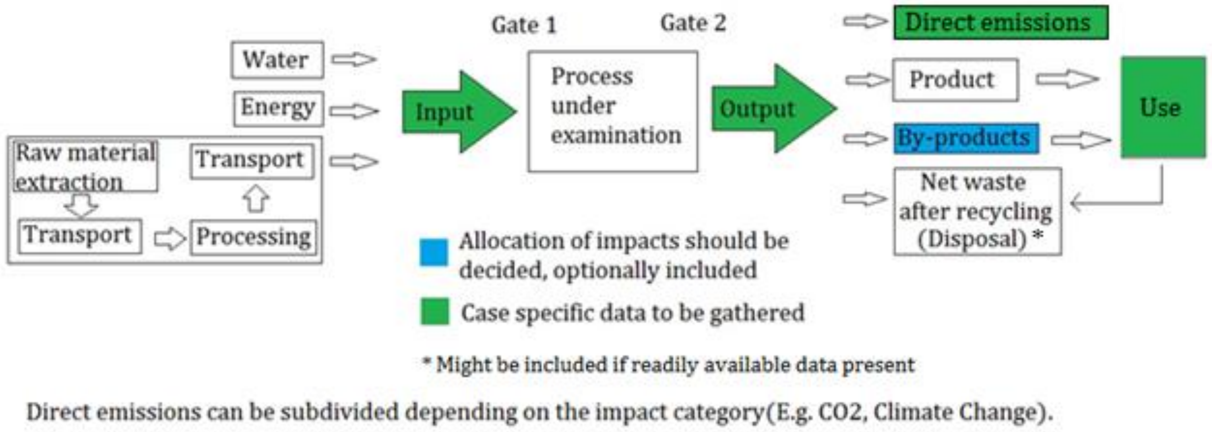


Fig. 6.4. Life Cycle Stages simplified diagram.

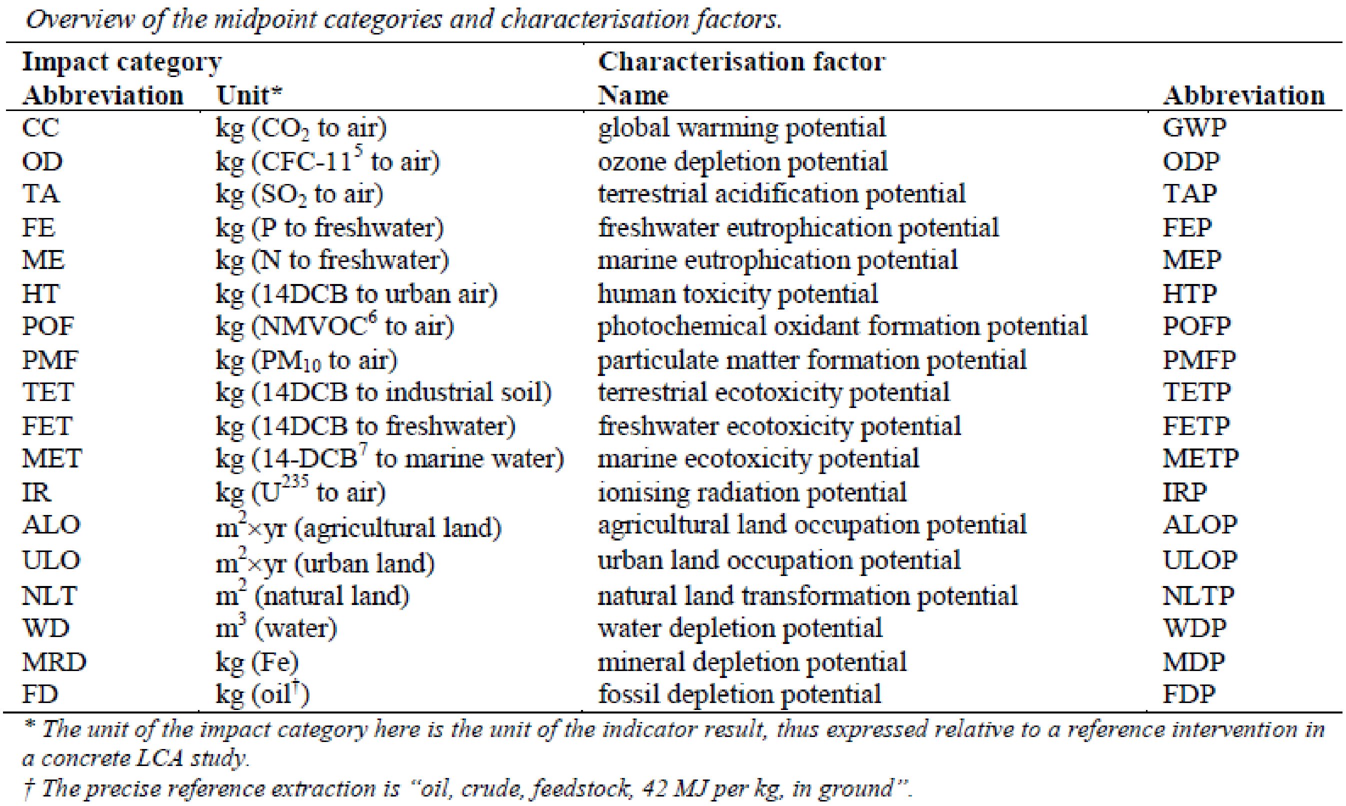
Note: A by-product is the output from a joint production process that is minor in quantity and/or economic value when compared to the main products.

In cases where some part of LCI cannot be found in the LCI database, according to ILCD handbook (http://publications.jrc.ec.europa.eu/repository/bitstream/JRC48157/ilcd_handbook-general_guide_for_lca-detailed_guidance_12march2010_isbn_fin.pdf), all the missing data should be documented in detail and marked as "missing important" or "missing unimportant" to be considered in the decision stage. The importance depends on the amount and hazardous properties of the missing substance. Data gaps for toxicity characterization factors for humans and the environment can be filled with different methods. In the project the USETox methodology will be used. In neither situation there will be a direct collection of data beyond the defined scope of the LCA (but if there is already available data, it can be used). Industry average data will be used from LCI databases (e.g. Ecoinvent).

6.2 Guidance for indicator derivation and impact assessment

After the Life Cycle Inventory, all impacts are calculated in terms of impact indicators by using appropriate methodologies, which is incorporated in the LCA software (for project purposes the SimaPro 8.0 will be used, which includes the Recipe methodology). The units of the midpoint indicators can be seen in Table 6.2. Those midpoint indicators are calculated by using midpoint characterisation factors, which is usually in terms of equivalents of a reference substance (Table 6.1). Midpoint characterisation factors in terms of equivalents of a reference substance (Table 6.1) will be used as indicators for the project because of their relatively low uncertainty (ReCiPe Midpoint E methodology).

Table 6.1. Midpoint categories and characterisation factors (ReCiPe 2008, May 2013)



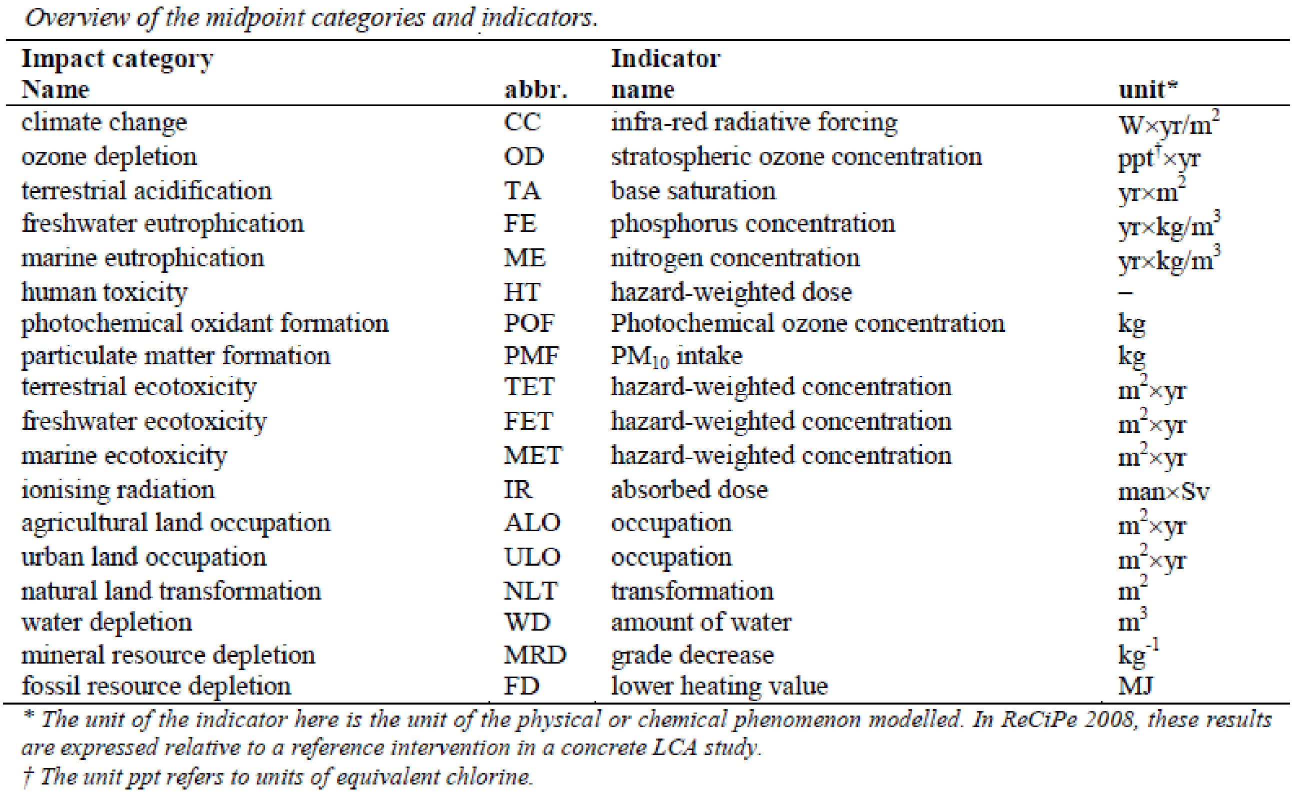
Overview of the midpoint categories and characterisation factors.

Impact category		**Characterisation factor**	
Abbreviation	**Unit***	**Name**	**Abbreviation**
CC	kg (CO_2 to air)	global warming potential	GWP
OD	kg (CFC-11[5] to air)	ozone depletion potential	ODP
TA	kg (SO_2 to air)	terrestrial acidification potential	TAP
FE	kg (P to freshwater)	freshwater eutrophication potential	FEP
ME	kg (N to freshwater)	marine eutrophication potential	MEP
HT	kg (14DCB to urban air)	human toxicity potential	HTP
POF	kg (NMVOC[6] to air)	photochemical oxidant formation potential	POFP
PMF	kg (PM_{10} to air)	particulate matter formation potential	PMFP
TET	kg (14DCB to industrial soil)	terrestrial ecotoxicity potential	TETP
FET	kg (14DCB to freshwater)	freshwater ecotoxicity potential	FETP
MET	kg (14-DCB[7] to marine water)	marine ecotoxicity potential	METP
IR	kg (U^{235} to air)	ionising radiation potential	IRP
ALO	m^2×yr (agricultural land)	agricultural land occupation potential	ALOP
ULO	m^2×yr (urban land)	urban land occupation potential	ULOP
NLT	m^2 (natural land)	natural land transformation potential	NLTP
WD	m^3 (water)	water depletion potential	WDP
MRD	kg (Fe)	mineral depletion potential	MDP
FD	kg (oil[†])	fossil depletion potential	FDP

** The unit of the impact category here is the unit of the indicator result, thus expressed relative to a reference intervention in a concrete LCA study.*

† The precise reference extraction is "oil, crude, feedstock, 42 MJ per kg, in ground".

Table 6.2. Midpoint categories and indicators (ReCiPe 2008, May 2013)



Overview of the midpoint categories and indicators.

Impact category Name	abbr.	Indicator name	unit*
climate change	CC	infra-red radiative forcing	W×yr/m^2
ozone depletion	OD	stratospheric ozone concentration	ppt†×yr
terrestrial acidification	TA	base saturation	yr×m^2
freshwater eutrophication	FE	phosphorus concentration	yr×kg/m^3
marine eutrophication	ME	nitrogen concentration	yr×kg/m^3
human toxicity	HT	hazard-weighted dose	–
photochemical oxidant formation	POF	Photochemical ozone concentration	kg
particulate matter formation	PMF	PM$_{10}$ intake	kg
terrestrial ecotoxicity	TET	hazard-weighted concentration	m^2×yr
freshwater ecotoxicity	FET	hazard-weighted concentration	m^2×yr
marine ecotoxicity	MET	hazard-weighted concentration	m^2×yr
ionising radiation	IR	absorbed dose	man×Sv
agricultural land occupation	ALO	occupation	m^2×yr
urban land occupation	ULO	occupation	m^2×yr
natural land transformation	NLT	transformation	m^2
water depletion	WD	amount of water	m^3
mineral resource depletion	MRD	grade decrease	kg^{-1}
fossil resource depletion	FD	lower heating value	MJ

** The unit of the indicator here is the unit of the physical or chemical phenomenon modelled. In ReCiPe 2008, these results are expressed relative to a reference intervention in a concrete LCA study.*

† The unit ppt refers to units of equivalent chlorine.

For the calculation of impact characterization factors at midpoint level, in ReCiPe method, the following equation is being used (Equ. 5):

Equ. 5: $I_m = \sum Q_{mi} m_i$

where

m_i is the magnitude of intervention i (e.g., the mass of CO_2 released to air);

Q_{mi} the characterisation factor that connects intervention i with midpoint impact category m;

I_m the indicator result for midpoint impact category m.

The overall impact per impact category (e.g. climate change, eutrophication, etc.) is calculated automatically by the software. The relevant indicators can be selected among the above mentioned indicators, after the implementation of LCIA. A general template for reporting purposes of the results without the normalisation step can be seen on Table 6.3.

Table 6.3. Template for reporting characterization at the midpoint level, without normalization step.

Midpoint category	**Value**	**Unit**
CC	*To be inserted by LCA practitioner*	kg (CO_2 to air)
OD	*To be inserted by LCA practitioner*	kg (CFC-11 to air)
TA	*To be inserted by LCA practitioner*	kg (SO_2 to air)
FE	*To be inserted by LCA practitioner*	kg (P to freshwater)
ME	*To be inserted by LCA practitioner*	kg (N to freshwater)
HT	*To be inserted by LCA practitioner*	kg (14 DCB to urban air)
POF	*To be inserted by LCA practitioner*	kg (NMVOC to urban air)
PMF	*To be inserted by LCA practitioner*	kg (PM10 to air)
TET	*To be inserted by LCA practitioner*	kg (14 DCB to soil)
FET	*To be inserted by LCA practitioner*	kg (14 DCB to freshwater)
MET	*To be inserted by LCA practitioner*	kg (14 DCB to marine water)
IR	*To be inserted by LCA practitioner*	kg (U 235 to air)
ALO	*To be inserted by LCA practitioner*	m^2xyr (agricultural land)
ULO	*To be inserted by LCA practitioner*	m^2xyr (urban land)
NLT	*To be inserted by LCA practitioner*	m^2 (natural land)
WD	*To be inserted by LCA practitioner*	m^3 (water)
MD	*To be inserted by LCA practitioner*	kg (Fe)
FD	*To be inserted by LCA practitioner*	kg (oil)

A step by step flow chart guide of the implementation of simplified LCA for the project is as follows (Figure 6.5):

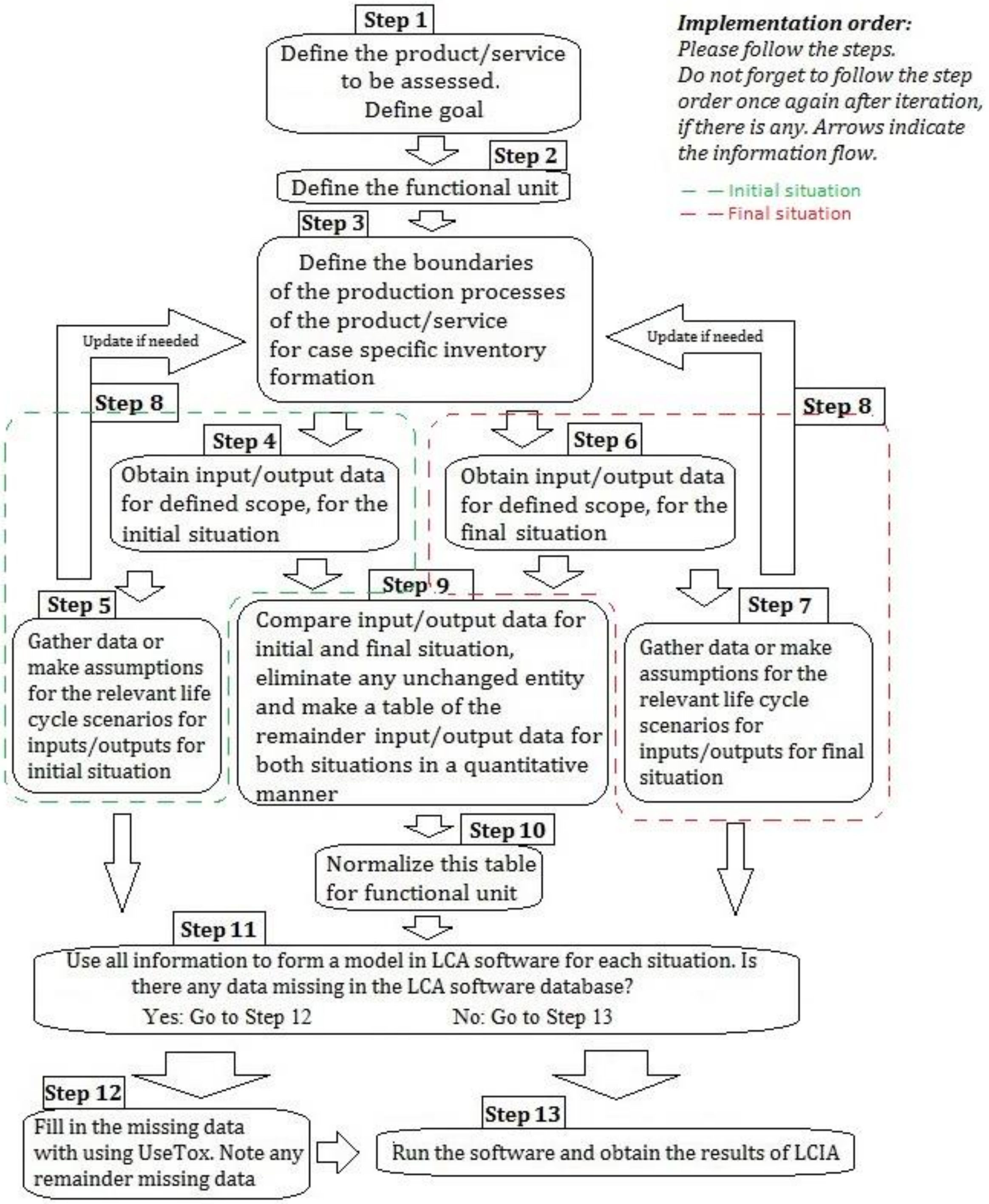


Fig. 6.5. Detailed step by step guidance for the implementation of simplified LCA.

Defining the goal (Step 1) and the functional unit (Step 2)

Step 1: Goal definition should be written as specific as possible, an example: “Product X of company C uses hazardous chemical Y in its production, the goal of this LCA is to assess changes in environmental impact of substitution of the hazardous chemical Y, with chemical Z.”

Step 2: The quantitative definition of a product’s functional unit should refer to technical standards wherever possible and appropriate. Harmonized standards under ISO should be preferred for this purpose wherever available. Examples: The amount of paint in kg needed to cover 1 m^2 outdoor wall according to standard XYZ (under defined weather conditions) with a red color (color code XYZ) for 10 years. A bottle which is able to contain and preserve 0,5 lt of pasteurized milk for at least two weeks. Etc…

Defining the boundaries for case specific inventory (Step 3)

Step 3: Before gathering any case specific inventory (Input/output data for the processes under examination), scope of the processes under examination should be clearly defined. This usually will be defined as the process boundaries of the companies that is producing the product/service and the use phase of the product/service. This boundaries, if found necessary in the following steps, can be modified and extended (in Step 8) to include the disposal phase of the product for initial and final situation.

Gathering data or making assumptions on life cycle scenarios (Step 4 and Step 5/Step 6 and Step 7)

Step 4: In Step 4, all the input/output data (Including energy) and amount of product produced for the initial situation should be gathered from the company (Over the period of 1 year) and if necessary from other sources (If the boundaries have been extended from the company boundaries). One important point is, the origin of input sources (Where is the inputs coming from? The water is drawn from a well, or a public pipe? Does the input chemicals produced in Europe, and which country? Is the company using a recycled material as input (When the information is easily available)? Etc…) and output paths (Where it is released (After end of pipe technologies if any), to air, to freshwater, to marine water, in detail, where is it going?) should be noted in detail whenever possible in the input/output table. After all the iterations and updates have been completed, all of the same type of input/outputs in Step 4 should be aggregated for initial situation and a table should be formed, taking into account of the differences of the release compartment (E.g. Air, freshwater) or input source. We will assume that all the changes in the company is due to substitution. Here is a list of all the data needs to be collected:

- All inputs/outputs of the production processes over 1 year period and the amount of product produced over the same 1 year period in the company that we are working with (Who produces the product). The input data (with CAS numbers if relevant) should be detailed and include origin (e.g. made in Poland, e.g. for water, extraction is from ground well in Lithuania), production method, amount of the inputs (Preferably in kg). The output data (with CAS numbers if relevant) should be detailed and include the emission department (e.i. air, freshwater, marine water, industrial soil, agricultural soil), and amount of the output (Preferably in kg).
- All direct emissions from the use phase should be noted in detail (with CAS numbers if relevant) and should include the emission department (e.i. air, freshwater, marine water, industrial soil, agricultural soil), and amount of the output (Preferably in kg). This data will be normalized to the total products produced over 1 year period and will be aggregated with the

other input/output data by taking into account the differences in source/release compartment, type of substance and initial/final situation.

- During the production in the company, if there is any waste related to the production of the product (i.e. process waste), the waste composition (with CAS numbers if relevant), amount (Preferably in kg) and disposal scenario should be noted whenever available. This should be done over the same 1 year period.
- After the use phase, if disposal scenario is known for the product or product components (Product components to be specified in detail; composition of the product component with CAS no. and weight distribution (Preferably in kg)), it should be noted. This should be done over the same 1 year period.

Attention should be given not to duplicate the same data. Also, uncertainties should be noted (e.g. maximum X, minimum Y), if there is any, for each piece of data.

At the end of the Step 4, the obtained table should be aggregated (By taking into account the uncertainties) within itself, by taking into account the differences in source/release compartment and type of substance, after making sure that the amounts are normalized to 1 year of production.

Step 5: In Step 5, other relevant data for the initial situation should be gathered if necessary about the life cycle of the product. The difference of Step 5 from Step 4 is that in Step 5 assumptions are being made instead of noting measured or known values. Such as, what are the emissions during the use phase (Use phase emissions and all other input/output data should be accounted for the total amount of product produced during the 1 year period. If this is calculated for 1 unit of product, it should be multiplied by the total number of products produced within this 1 year period), is it known from other information sources which percent of the product ends up where (E.g. 40% landfill, 30% recycled, 30% incineration)?

Step 6: This step is same as Step 4, except it will be implemented for the final situation. At the end of the Step 6, the obtained table should be aggregated (By taking into account the uncertainties; adding Min. values with Min. and Max. values with Max.) within itself, by taking into account the differences in source/release compartment and type of substance, after making sure that the amounts are normalized to 1 year of production.

Step 7: This step is same as Step 5, except it will be implemented for the final situation.

Step 8: If any case specific information found in Steps 5 and 7, Step 3 should be updated accordingly if necessary.

Note: In any step, if a range of input/output value is known instead of an exact value, it can be written in the table as such: Max value: X, Min value: Y. Only one of the values will be selected by using precautionary principle, worst case scenario. E.g. It is known that emission of substance X to environmental compartment C from use phase is Max: Y, Min: Z.

Filtering input/output data (Step 9)

Step 9: Any value (Including uncertainties; Min. and Max. values) that has changed in the input/output between the initial and the final situation (Tables from Step 4 and Step 6) should be carried to the next step, for both situations. This means, only the values that are different among the two tables that are the outcome of Step 4 and Step 6 will be carried to Step 10. Again, the type of input/outputs, including the information on the release compartment or the input source should be taken into account. As an example: Among the tables from Step 4 and Step 6, emission of substance X to the environmental compartment Y has been decreased, input of low voltage electricity has been increased, etc. hence those information will be carried to the next step for both situations; a table will be made including the emission of substance X to the environmental compartment Y for initial situation, and for final situation. Electricity input will be included in this table for the initial and final situation, with a note that the source is low voltage electricity.

Normalization of filtered input/output data for functional unit (Step 10)

Step 10: The information from Step 9 should be normalized to the functional unit. This is an easy and straight forward step. E.g. If the company is using X amount of electricity to produce Y amount of product, how much electricity is needed to produce the functional unit. Another example, if the company is using X amount of substance Y from a defined source to produce Z amount of product, how much substance Y from the same source is needed to produce the functional unit.

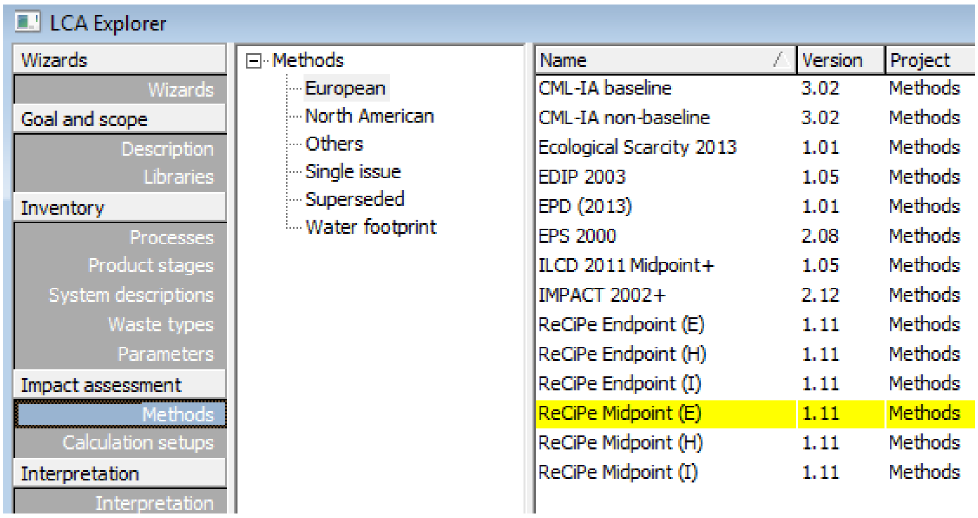
The outcome of this step would look like this (Table 6.4):

Table 6.4. Outcome of Step 10, input/output values normalized to functional unit.

Input/output per functional unit initial situation				**Input/output per functional unit final situation**			
Inputs	From	Outputs	To	Inputs	From	Outputs	To
0,01 kg substance X	Lithuania, LT	0,03 kg CO_2	Air	0,02 kg substance Y	Estonia, EE	0,032 kg CO_2	Air
0,5 L water	Ground water, well, LT	0,3 kg substance A	Landfill, LT	0,51 L water	Ground water, well, LT	Max: 0,7 kg Min: 0,4 kg substance C	Fresh water, river
0,008 kWh electricity	Low voltage, LT	0,04 kg substance B	Incineration, LT	0,007 kWh electricity	Low voltage, LT		
Etc…				Etc…			

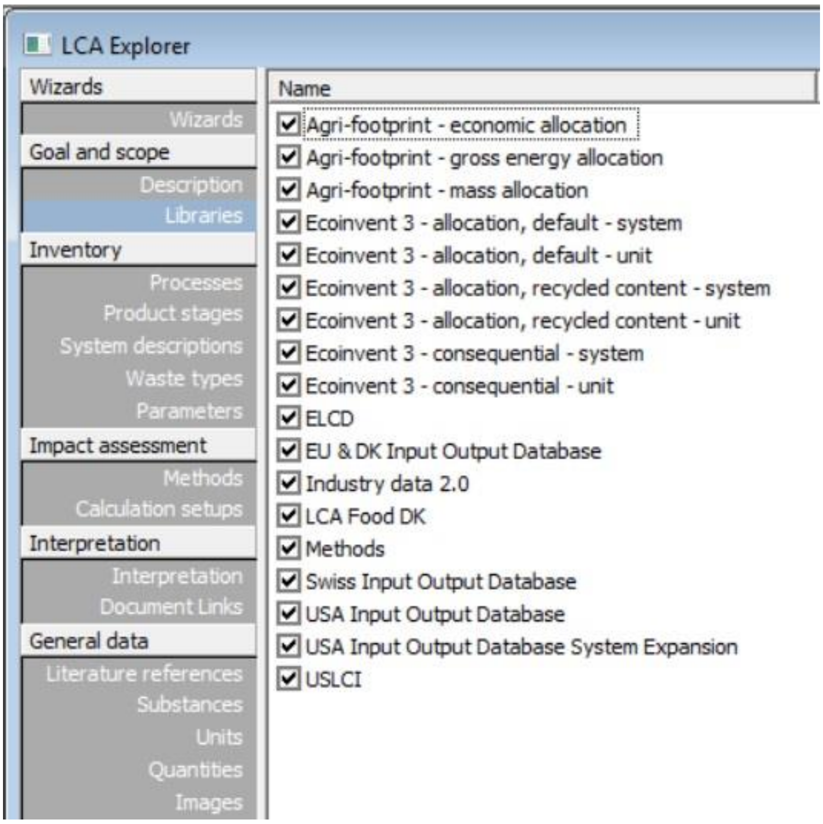
Forming the model in LCA software (Step 11)

Step 11: All the relevant information from Step 10 and Steps 5 and 7 will be used to model both situations. Worst case values will be decided at this step, if there is any uncertainties. The software that will be used is Simapro 8 and it includes databases for industry average values throughout EU, country specific and world average. Allocation by economic value as “Allocation Default System Model” (Alloc Def) would be used as allocation method.



Name	Version	Project
CML-IA baseline	3.02	Methods
CML-IA non-baseline	3.02	Methods
Ecological Scarcity 2013	1.01	Methods
EDIP 2003	1.05	Methods
EPD (2013)	1.01	Methods
EPS 2000	2.08	Methods
ILCD 2011 Midpoint+	1.05	Methods
IMPACT 2002+	2.12	Methods
ReCiPe Endpoint (E)	1.11	Methods
ReCiPe Endpoint (H)	1.11	Methods
ReCiPe Endpoint (I)	1.11	Methods
ReCiPe Midpoint (E)	1.11	Methods
ReCiPe Midpoint (H)	1.11	Methods
ReCiPe Midpoint (I)	1.11	Methods

LCIA methods, screenshot of SimaPro 8. ReCiPe Midpoint (E) will be used for the purposes of this project as mentioned before.



Name

- ☑ Agri-footprint - economic allocation
- ☑ Agri-footprint - gross energy allocation
- ☑ Agri-footprint - mass allocation
- ☑ Ecoinvent 3 - allocation, default - system
- ☑ Ecoinvent 3 - allocation, default - unit
- ☑ Ecoinvent 3 - allocation, recycled content - system
- ☑ Ecoinvent 3 - allocation, recycled content - unit
- ☑ Ecoinvent 3 - consequential - system
- ☑ Ecoinvent 3 - consequential - unit
- ☑ ELCD
- ☑ EU & DK Input Output Database
- ☑ Industry data 2.0
- ☑ LCA Food DK
- ☑ Methods
- ☑ Swiss Input Output Database
- ☑ USA Input Output Database
- ☑ USA Input Output Database System Expansion
- ☑ USLCI

Industry average databases included in SimaPro 8.

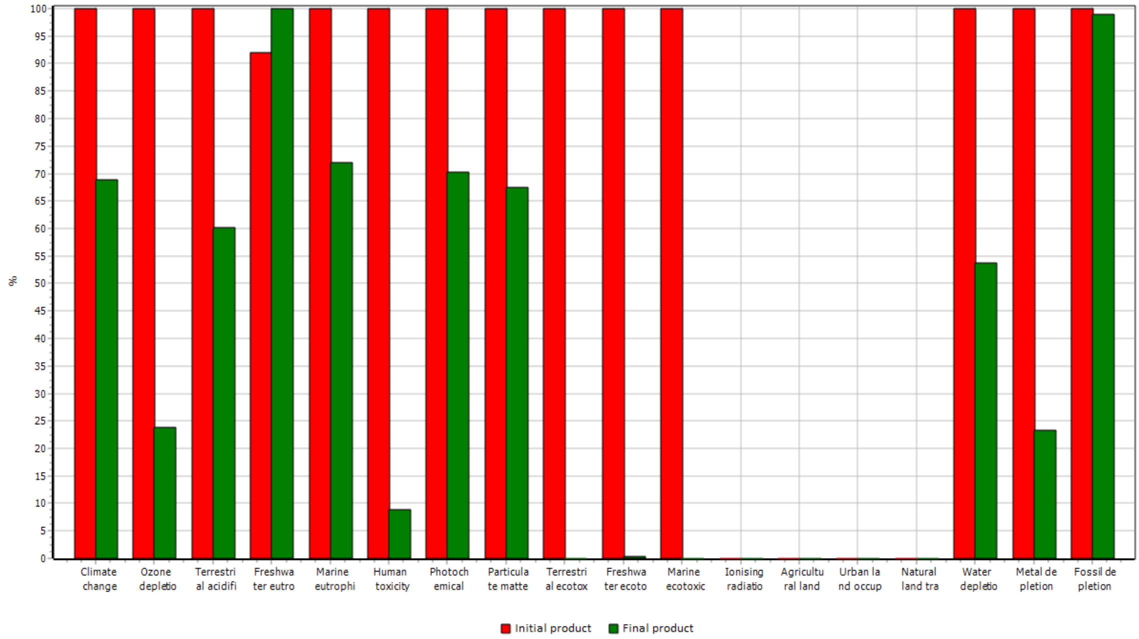
Dealing with the missing data (Step 12)

Step 12: UseTox can be used to fill in the gaps in ecotoxicity and human toxicity characterization factors whenever the toxicity data and physical properties are available. It is possible to manually enter physicochemical and toxicity properties to USEtox and have the characterization factors. (USEtox team experts guides as: For implementing the USEtox factors yourself in SimaPro, the starting point are the results files from USEtox in XLSX format. These can be "saved as" different formats like e.g. sheet-by-sheet in CSV format and can be used in SimaPro). All the remainder missing data should be noted in detail and labelled as “missing important” or “missing unimportant”. Any missing toxicity data should be labelled as “missing important” for precautionary reasons. If the range of uncertainty in any of the missing data is known, it is possible to use the worst case, again considering precautionary principle.

Note: Any assumptions made (Including the use of worst case scenario in detail, for which input/outputs worst case has been selected and what is the uncertainty range) and sources of data should be noted clearly for each step.

6.3. Interpretation of the results from LCA software

The LCA results for characterization are shown below in the Figures 6.6 and Table 6.5 for the given example:



Method: ReCiPe Midpoint (E) V1.11 / Europe Recipe E / Characterization
Comparing 1 kg 'Initial product' with 1 kg 'Final product';

Fig. 6.6. Graph representation of SimaPro 8.0.4 results for initial and final product, with relative to each other in each impact category.

Table 6.5. Table representation of SimaPro 8.0.4 results for initial and final products.

Impact category	Unit	Initial product	Final product
Climate Change	kg CO_2 eq	1,55	1,07

Ozone depletion	kg CFC-11 eq	2,88E-11	6,86E-12
Terrestrial acidification	kg SO_2 eq	0,00621	0,00373
Freshwater eutrophication	kg P eq	1,46E-7	1,59E-7
Marine eutrophication	kg N eq	0,000115	8,31E-5
Human toxicity	kg 1,4-DB eq	0,00582	0,000517
Photochemical oxidant formation	kg NMVOC eq	0,00344	0,00242
Particulate matter formation	kg PM10 eq	0,00194	0,00131
Terrestrial ecotoxicity	kg 1,4-DB eq	0,000494	3,64E-7
Freshwater ecotoxicity	kg 1,4-DB eq	0,000193	6,6E-7
Marine ecotoxicity	kg 1,4-DB eq	0,745	0,000197
Ionising radiation	kBq U 235 eq	X	X
Agricultural land occupation	m^2xyr	X	X
Urban land occupation	m^2xyr	X	X
Natural land transformation	m^2	X	X
Water depletion	m^3	0,000629	0,000338
Metal depletion	kg Fe eq	0,000476	0,000111
Fossil depletion	kg oil eq	1,48	1,46

These results are the same entity as in Table 6.1. After the characterization, these results should be normalised (Table 6.6) to the impact of the average EU citizen, and only then, environmentally significant indicators can be selected accordingly.

Results after normalisation (Fig. 6.7):

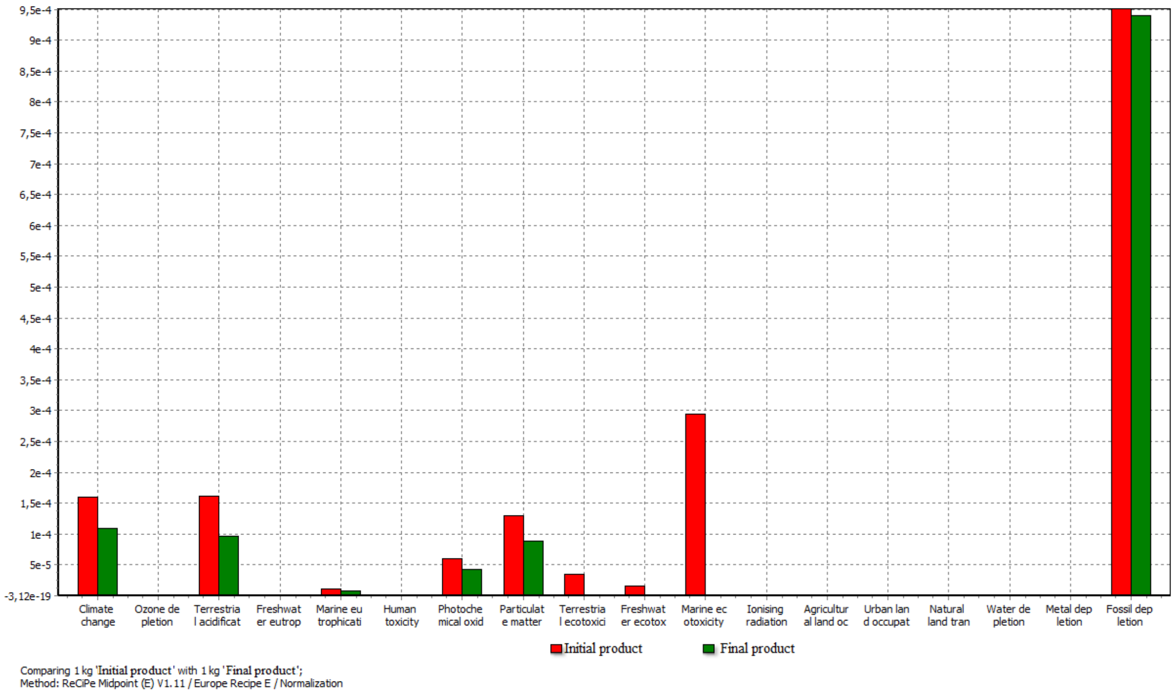


Fig. 6.7. Graph representation of SimaPro 8.0.4 results for initial and final product, after normalisation. The relative importance of the environmental impacts can be seen on the graph.

Table 6.6. Table representation of SimaPro 8.0.4 results for initial and final products, after normalisation.

Impact category	Unit	Initial product	Final product
Climate Change		0,0016	0,00011
Ozone depletion		1,31E-9	3,11E-10
Terrestrial acidification		0,000162	9,71E-5
Freshwater eutrophication		3,52E-7	3,83E-7
Marine eutrophication		1,14E-5	8,21E-6
Human toxicity		1,3E-6	1,16E-7
Photochemical oxidant formation		6,06E-5	4,26E-5
Particulate matter formation		0,00013	8,79E-5
Terrestrial ecotoxicity		3,53E-5	2,6E-8
Freshwater ecotoxicity		1,65E-5	5,66E-8
Marine ecotoxicity		0,000294	7,79E-8

Ionising radiation		X	X
Agricultural land occupation		X	X
Urban land occupation		X	X
Natural land transformation		X	X
Water depletion		x	x
Metal depletion		6,66E-7	1,55E-7
Fossil depletion		0,000951	0,000941

How to choose relevant environmental impact indicators? As an example, it can be seen in Figure 6.7 and Table 6.6 (Hypothetical outcome of the LCIA), fossil depletion, marine ecotoxicity, climate change, terrestrial acidification, particular matter formation, photochemical oxidation, terrestrial ecotoxicity and freshwater ecotoxicity is significant for at least one of the products. Hence, those can be selected as relevant indicators for this example.

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ANNEX I

Benchmarking the initial environmental situation

Emissions of hazardous substances leave a trace in various compartments in environment. An assessment of environmental concentration by the FitForReach project is primarily linked to the environmental quality standards (EQS) for the substances in surface waters, due to the potential for adverse impacts upon human and ecosystem health (EEA, 2011). Based on the substance intrinsic chemical properties, we have indicated four main groups of substances: phthalates, organic tin compounds, phenols and bisphenols to reflect on environmental concentration in Latvia, Lithuania and Estonia. However, data on environmental concentration for the phthalates, organic tin compounds, phenols and bisphenols are scarce. Scattered information was possible to gather form the screening results of previous project based activities and measurements in the frame of national monitoring programme (Table I.1). The EQS were exceeded in several sampling locations. This would indicate an emerging concern towards releases of the hazardous substances to waters; however, the current data are pre-mature to elaborate a systematic assessment.

Table I.1. Overview of environmental concentration of substances in Latvia (LV), Lithuania (LT) and Estonia (EE)[12]

Group of substances	Assessment of substances in environment
Phthalates	DINP – no data found Other phthalates: LV: Concentration of DEHP in water bodies did not exceed annual average environmental quality standard (EQS) of 1.3 ug/L in 2012 (Kalvane & Veidemane, 2013), and in 2014 (LEGMC, 2015). Relatively high DEPH concentration has been measured in sediments (440 ug/kg in water body *Berze*) (LEGMC, 2015). LT: DEHP occurrence has been found in water (up to 3.85 ug/L) and in sediments (22000 ug/kg) (Dudutyte *et.al*, 2011). EE: DEHP has been measured in river water (0.28 ug/L in the *River Jagala*) (Roots and Nommsalu, 2011).
Organic tin compounds	Dibutilyn dilaurate – no data found Other organic tin compounds: LV: In 2014, the concentration of Tributyltin (TBT) in two water bodies has been close to maximum allowable concentration (MAC) of 0.0015ug/L (LEGMC, 2015).

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[12] We do not expect seeing any changes to the occurence of the substances due to the project activities.

	LT: In surface waters, the concentration of TBT downstream the bigger towns exceeded the EQS (up to 0.004 ug/L in *Nemunas*, and in *Nevezis*) (Dudutyte *et.al*, 2011). TBT concentration in riverine sediments (1.6 -585 ug/L), higher concentration found in the port territory (12.8-2400 ug/kg in sediments of Klaipeda channel and in the port territory) (Dudutyte *et.al*, 2011). EE: Degradation compounds of TBT (as DBT and MBT) were found in relatively high contents, but the concentration of TBT remained below the limit of quantification (LOQ) of 0.0002 ug/L (in the Rivers *Narva*, *Kasari* and *Keila*) (Roots and Nommsalu, 2011).
Phenols	Data available for nonylphenol : LV: In 2014, the concentration of Nonylphenol in surface waters did exceed EQS (0.3 ug/L) and MAC (2 ug/L) (LEGMC, 2015). LT: Nonylphenol is suggested to be included in a monitoring programme (2011-2017) due to preliminary indication of presence in surface water and sediments (Dudutyte *et.al*, 2011).
Bisphenols	Data available for Bisphenol A : LV: In 2012, the concentration of Bisphenol A has been measured in sediments (25.4 ug/kg (dry weight) in lake *Murati*, and 11.1-4.66 ug/kg (dry weight) at other sampling sites in *Gauja/Koiva*) (Kalvane & Veidemane, 2013). LT: Bisphenol A is suggested to be included in a monitoring programme (2011-2017) due to preliminary indication of presence in surface water and sediments (Dudutyte *et.al*, 2011).