KAUNAS UNIVERSITY OF TECHNOLOGY
UNIVERSITY OF BOLOGNA

SEMIH OGUZDJAN

ENVIRONMENTAL IMPACT ASSESSMENT MODEL FOR SUBSTITUTION OF HAZARDOUS SUBSTANCES BY USING LIFE CYCLE APPROACH

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Technological Sciences, Environmental Engineering (T 004)

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Scientific Supervisors:

Prof. Dr. Jolanta DVARIONIENĖ (Kaunas University of Technology, Technological Sciences, Environmental Engineering, T 004);

Assoc. Prof. Dr. Alessandro TUGNOLI (University of Bologna, Italy, Technological Sciences, Environmental Engineering, T 004).

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SEMIH OGUZDJAN

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Doc. dr. Alessandro TUGNOLI (Bolonijos universitetas, technologijos mokslai, aplinkos inžinerija, T 004).

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Abbreviations

AoP	Areas of Protection
BFRs	Brominated Flame Retardants
CBA	Cost Benefit Analysis
CMR	Carcinogenic, Mutagenic and Reprotoxic
CTUh	Comparative Toxic Unit for human
DALYs	Disability Adjusted Life Years
DfE	Design for the Environment
DNEL	Derived No Effect Level
ERCs	Environmental Release Categories
GHS	Globally Harmonized System of Classification and Labelling of Chemicals
LCA	Life Cycle Assessment
LCC	Life Cycle Costing
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCIT	Life Cycle Inherent Toxicity
LCRA	Life Cycle Risk Assessment
LCT	Life Cycle Thinking
MCDA	Multi-criteria Decision Analysis
MFA	Material Flow Analysis
MSDS	Material Safety Data Sheet
PBT	Persistent, Bio-accumulative and Toxic
PNEC	Predicted No Effect Concentration
POPs	Persistent Organic Pollutants
PROCs	PROcess Categories
QRA	Quantitative Risk Assessment
QSAR	Quantitative Structure-Activity Relationship
RA	Risk Assessment
RCR	Risk Characterization Ratio
SDS	Safety Data Sheet
SLCA	Social Life Cycle Assessment
SMEs	Small and Medium-sized Enterprises
SVHC	Substances of Very High Concern
VOCs	Volatile Organic Compounds
vPvB	very Persistent and very Bio-accumulative
WE_DALYs	Work Environment Disability Adjusted Life Years
WE-CFs	Work Environment Characterization Factors
YLD	Years Lost due to Disability
YLL	Years of Life Lost

Glossary

Areas of Protection	entities to be protected such as the natural environment, human health, and natural resources
Effect factors	cancer/non-cancer disease cases per kg intake of a chemical
Intermediate flows/chemicals	chemical flows among life cycle stages
Life Cycle Assessment	a method to assess environmental impacts associated with all the stages of a product’s life
Life Cycle Inventory	input-outputs of a product system concerning the life cycle of the product
Life Cycle Impact Assessment	a method for linking life cycle inventory to the environmental impacts
Material Flow Analysis	input-outputs of a system
Small and Medium sized Enterprises	enterprises with 250 or fewer staff
Substances of Very High Concern	CMR, PBT, vPvB, endocrine disruptor substances or substances with similar severity of concern
Technosphere	sphere or realm of human technological activity
Volatile organic compounds	organic substances with vapor pressure 0.01 kPa or greater at room temperature

Introduction

Research relevance

Environmental pressures (such as greenhouse gas emissions, release of high toxicity chemicals into the environment, etc.) related to industrial activities are a concern for the well-being of the environment and humans. Search for less toxic chemical alternatives, which is seen as a green chemistry effort concerning the life cycle of products, needs to consider the changes in the overall production system stemming from a decision on chemical substitution in the company.

Exponential increase in global atmospheric greenhouse gas concentrations (Keeling, Keeling 2017) can be used to conclude (by using the proportionality of energy usage and environmental impacts (Huijbregts *et al.*, 2010; Huijbregts *et al.*, 2006)) that global emissions of hazardous chemicals that are not being substituted or phased out are also increasing exponentially in the environment. The current substitution practices in SMEs, as driven by the EU regulations, primarily focus on reducing the carcinogenic, mutagenic and reprotoxic (CMR), persistent, bio-accumulative and toxic (PBT) or very persistent and very bio-accumulative (vPvB) substances at the company level, without much focus on the life cycle impacts of these decisions. However, it should be clear that local decisions are not the optimum path towards reduction of the overall impacts, and they potentially decrease the substitution efficiency (reduction in environmental impacts per resources spent) and waste resources without much reduction in environmental impacts. Life cycle assessment (LCA) is a method used to evaluate the environmental impacts associated with all the stages of a product's life cycle. These stages include raw material extraction, materials processing, manufacture, distribution, use, recycling (if any), and disposal. LCA is being used for many purposes, such as ecolabelling, product improvement and product comparison in terms of their environmental impact (EU, 2010a; Lehtinen *et al.*, 2011; Borghi, 2013). As being state of the art, the implementation of LCA has been standardized to some degree with the development of ISO 14040/44 Standards and the subsequent publication of guidance, such as the International Reference Life Cycle Data System (ILCD) handbooks (EU, 2010a). Nevertheless, many problems exist in almost each step of the LCA application that are waiting to be resolved. One of these problems is the expertise needed to conduct the traditional LCA studies (Iraldo *et al.*, 2015). Due to this limitation, in companies where expertise is lacking, environmental impacts associated with the complete life cycle of a product are often ignored during decision making in terms of alternatives assessment. This is particularly important as small and medium-sized enterprises (SMEs) constitute a major part of the global production (Hussey, Eagan, 2007; Baranova, Paterson, 2017); yet, the regulatory requirements are set only for the major issues while ignoring the fact that the aggregation of many small impacts may lead to a big impact.

This is particularly problematic when chemical alternatives assessments need to be performed due to regulatory mandates. One of such mandates in EU is the REACH regulation. The REACH regulation came into force in 2007 as a major regulatory driver for the chemicals substitution in the European Union, which makes substitution of the most hazardous substances (substances of very high concern) inevitable whenever a less hazardous alternative is present (European Chemicals Agency [ECHA], 2007). To address the need for a framework describing how to progress with the alternatives assessment, the literature provides a wide range of options for a variety of assessor types (from SMEs to government bodies) with varying resources. In these chemical alternatives assessment frameworks, LCA is optional and usually serves for assessors with sufficient time and resources. Occupational safety, as well as accidental and fugitive emissions along the whole life cycle, are also often neglected. In this context, fugitive emissions are unintended releases, such as gas leaks from pipeline connections.

Therefore, appropriate integration of novel methodologies into already available chemical alternatives assessment frameworks that will enable the assessors with limited resources to evaluate the impacts of their decisions on the environment as well as on the workers at least for part of the life cycle of their products is necessary. Also, when possible, error reduction methods should be in place in case of missing information or inexpert errors. Throughout the thesis, ‘expert’ means an assessor who can select the correct parameters related to the environmental/human health impacts to the extent of state of the art.

This doctoral thesis aims to develop an environmental impact assessment model that enables integration of life cycle environmental impacts and life cycle occupational safety considerations into alternatives assessment frameworks to be used by companies with varying degrees of resources.

Aim and tasks of the research

The aim of the research is to develop an environmental impact assessment model for the substitution of hazardous substances by using the life cycle approach.

Tasks:

1. To analyze the existing research on the environmental impact assessment of the substitution of hazardous substances.
2. To develop a model for the environmental impact assessment of substitution of hazardous chemicals in industrial companies.
3. To apply the developed model to selected company cases and evaluate the feasibility of its application.
4. To explore possible improvements on the wider use of assessments by SMEs.

Key thesis

“The developed environmental impact assessment model enables companies to assess life cycle environmental impacts with a streamlined scope including substances of very high concern, fugitive and accidental emissions, as well as life cycle occupational safety concerns.”

Research object and methodology

The research object is hazardous substances.

The research steps are as follows: a systematic literature review intended to identify problems and tools/methods used in the area of chemical alternatives assessment, followed by the examination of the suitability of relevant methods obtained from the literature, and integration of these methods into the proposed environmental impact assessment model. Additionally, we intend to propose an error reduction method and an expert systems approach potentially to be used by SMEs.

Scientific novelty

The main scientific novelty of this research is the developed environmental impact assessment model that for the first time enables companies with limited resources to perform simplified life cycle impact assessments concerning environment and occupational safety, and incorporates life cycle accidental and fugitive emission impacts in these assessments. Also, for the first time in the environmental impact assessment literature, an error reduction and data gap management method based on the ‘wisdom of the crowds’ effect has been proposed. The developed model has been applied to real case studies concerning the substitution of hazardous substances. In addition, for the first time, an inter-company expert system has been proposed with a novel ‘combined total functional demand’ to increase the applicability of the model by inexpert assessors.

Practical value

The developed model can potentially be used by any industrial company to help to reduce the environmental impacts and occupational safety risks of production chains. The proposed model also renders SMEs more competent in evaluating their life cycle environmental impacts. The proposed error reduction method can be used to reduce errors in environmental impact results, as well as to fill in the data gaps in certain areas, such as life cycle inventories.

Approval of the Doctoral Dissertation

Four papers have been published in journals referred in ‘Clarivate Analytics-Web of Science’ database with impact factors, one paper has been published in a journal indexed in ‘Clarivate Analytics-Web of Science’ database without the current impact factor (the last impact factor was from 2010), and one paper has been published in other international scientific journals; in total, six papers fully covering this thesis have been presented.

Structure and contents of the dissertation

The dissertation consists of an introduction, five main chapters, conclusions, references, and supplementary materials.

The first chapter contains a systematic literature review in the fields of regulations, environmental issues caused by hazardous substances, chemical alternatives assessment, life cycle occupational safety, synergistic effects of carcinogenic substances, statistical approaches for error reduction, and expert systems used in environmental impact assessment. Following the literature review, the research gaps have been identified. The second chapter presents the research methodology and explanation of the justification of the research methodologies in use. The third chapter delivers preliminary evaluation of life cycle occupational safety methods. The fourth chapter contains an explanation of the proposed environmental impact assessment model, a statistical method for error reduction, and an expert systems approach. The fifth chapter presents the description of four different company cases from countries in the Baltic region and the main results of the model application in a fabric bleacher company, a polyurethane foam production company, a metal processing company and a floor coating company, as well as the results of the application of the statistical error reduction method. Finally, conclusions and recommendations are presented. The dissertation is comprised of 184 pages, including 26 figures and 84 tables. The list of references contains 218 sources.

1. Literature Review

1.1. Regulations concerning substitution of hazardous substances in EU

Chemical substitution is a fundamental part of cleaner production; hence it is needed for bringing the technosphere closer to a sustainable state. Due to the increasing concerns about the impact of our industrial activities, in the U.S., starting with the ‘Massachusetts Toxics Use Reduction Act of 1989 (TURA)’ (Ellenbecker, Geiser, 2011), the reduction of toxic chemicals has been taken into the law system. In EU, with the ESR (Existing Substances Regulation; one of former European Regulations on Chemicals, before the REACH Regulation) applicable from 1994 to 2007, four priority substances lists were published including 141 hazardous substances (ECHA, 2016). Many actions have been taken to eliminate the ‘obvious’ substances of concern of its time, such as the Stockholm Convention that addresses POPs (Persistent Organic Pollutants) (Hagen, Walls, 2005). The REACH regulation came into force in 2007 as a major regulatory driver for the chemicals substitution in the European Union, which makes substitution of the most hazardous substances, namely ‘substances of very high concern’ (SVHC), inevitable whenever a less hazardous alternative is present (ECHA, 2007). Potential inclusion of SVHC into the ‘candidate list’ is being done on case-by-case basis, with the help of Article 57 and Annex XIII to the REACH regulation which set out the description of SVHC substances as carcinogenic, mutagenic, reprotoxic (CMR), persistent, bio-accumulative and toxic (PBT), and very persistent and very bio-accumulative (vPvB) substances, endocrine disruptors, or substances with equivalent concern. Throughout the thesis, SVHC will be defined with these criteria of the REACH regulation, as a subset of hazardous substances. As a note, Annex XIII to the REACH regulation does not cover inorganic substances. Substances in the ‘authorization list’, as overseen by Annex XIV to the REACH regulation, need application for authorization by ECHA for their manufacturing, placing on the market or use. At this point, all suppliers of the substances that appear in the ‘authorization list’ are obligated to provide ‘safety data sheets’ (SDSs) to their customers overseen by Annex II to the REACH regulation. The application for authorization has a deadline, namely, the ‘latest application date’. Once a substance is on the ‘authorization list’, it is also given a ‘sunset date’, which determines a deadline for that substance to be used without authorization. Substances in the ‘restriction list’ are subject to restrictions in their manufacturing, placing on the market or use, as overseen by Annex XVII to the REACH regulation. Hence, the REACH regulation is a powerful driver for the substitution of SVHC substances in the EU, and, by default, also for those companies which want to export to the EU region.

1.2. Environmental and health problems caused by hazardous substances

Ecosystems as delicately balanced and enormously complex systems that evolved over millions of years are susceptible to disruption by any novel activity. Since the industrial revolution, the pressure on the natural balance has been increasing rapidly, and in most cases exponentially. This can be seen from many environmental observations. Arguably, the most famous example is the exponential increase in the global atmospheric greenhouse concentrations (Keeling, Keeling 2017) with dire consequences (Ciscar *et al*., 2018; Guldberg *et al*., 2018) if the ‘business as usual economic growth’ paradigm is being kept in place. The steady increase in concentrations of new chemical mixtures with unknown effects in the marine environment is getting to a point of critical concentration where effects are becoming observable as reported by Lehtonen *et al*. (Lehtonen *et al*., 2014). Endocrine disruptor substances in the environment (Annamalai, Namasivayam, 2015), risks from heavy metals (Govind, Madhuri, 2014), hazardous metals originating from electronic waste (Uchida *et al*., 2018; Garlapati, 2016) and risks from pharmaceuticals (Küster, Adler, 2014) are also a significant and increasing concern. Pharmaceuticals, biocides and disinfection by-products cause additional concern for the environment regarding their various effects, such as endocrine disruption and toxicity (Farre *et al*., 2008). A study examining the ‘traditional’ pollutants, such as polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), polybrominated biphenyl ethers (PBDEs), hexabromocyclododecane (HBCDD), toxic metals Cd, Hg and Pb, chlorinated dioxins and furans, alkylated PAHs and polyfluorinated compounds (PFC)s, concluded that their levels are a significant concern in many marine regions (Robinson *et al*., 2017).

Apart from the climate change, carbon dioxide emissions are becoming a significant problem causing ocean acidification (Doney *et al*., 2009). Ocean acidification affects the shell growth of plankton, benthic mollusks, echinoderms, and corals (Doney *et al*., 2009).

Terrestrial (soil) acidification is caused by deposition of acidifying compounds on soil leading to increased mobility of hazardous metals, biodiversity loss of plants, and to subsequent impacts on fauna (Azevedo *et al*., 2013).

Eutrophication is another major problem, mainly caused by nitrogen and phosphorus emissions predominantly from agriculture affecting water quality and biodiversity (Smith, Joye and Howarth, 2006).

Chlorofluorocarbons (CFCs), a stratospheric ozone depleting substance, in terms of use are on the rise once again as illegal activities have been taking place in Eastern China since 2012 (Montzka *et al*., 2018; Lin *et al*., 2019).

Tropospheric ozone formation by photochemical reaction of mainly nitrogen oxides (NO_x), carbon monoxide (CO), methane (CH_4), and volatile organic compounds (VOCs) is another concern impacting human and plant health (Kaur, 2016).

Bis(2-ethylhexyl) phthalate (DEHP), as a common plasticizer, raised concerns for its reprotoxic properties. According to Annex XVII of the REACH regulation, the use of DEHP and three other phthalates (namely, dibutyl phthalate (DBP), benzyl butyl phthalate (BBP), and diisobutyl phthalate (DIBP)) have been restricted in the EU for toys and childcare articles containing more than 0.1% of these chemicals cumulatively. This restriction will be extended to many other articles in July 2020 with a few exceptions, such as medical devices.

Bisphenol A (BPA) is another SVHC that is a concern due to its reprotoxic properties. BPA is a significant concern especially in the developmental stages during pregnancy as it causes various observable adverse effects. For the newborn and infants, canned baby formulas and mother's milk are some known exposure routes (Mendonca *et al*., 2014). In the EU, BPA is restricted from use in baby bottles due to these concerns. Another restriction will be in force starting from January 2020 for the use in thermal paper in a concentration equal to or greater than 0.02% by weight in order to limit the exposure of the unborn children of workers and consumers who handle the receipts (European Commission [EC], 2016).

Nonylphenol, a surfactant with suspected reprotoxicity, is another SVHC that has been restricted in various articles and mixtures, such as in detergents (ECHA, 2019b).

Endocrine disruptor substances, such as nonylphenol and BPA, cause various behavioral and physical changes in organisms including fish and mammals (Soares *et al*., 2008; Söffker and Tyler, 2012) contributing to biodiversity loss.

Hexabromocyclododecane (HBCDD), predominantly used in polystyrene foam for thermal insulation of buildings, raised concerns due to its persistent, bio-accumulative and toxic (PBT) properties and suspected reprotoxicity. The manufacture and use of this substance requires authorization by EU under Annex XIV of the REACH regulation (ECHA, 2019a). Another PBT substance bis(pentabromophenyl) ether (decaBDE), a type of PBDE that is being used as a flame retardant, was expected to be phased out from manufacture and use starting from March 2019 with a few exceptions (ECHA, 2019b).

Notifications of problematic substances by companies with their areas of usage in the EU region can be found on the “Data on Candidate List Substances in Articles” by ECHA. Also, the areas of usage of restricted substances under REACH regulation can be found on ECHA’s website (ECHA, 2007).

Although the substitution of SVHC substances is progressing, reductions in the life cycle emissions of other hazardous substances that are not listed as SVHC are not guaranteed and still have to be evaluated. The increase in the amount of these non-listed substances might overwhelm the decrease in the amount of the specific SVHC. If this is the case, the environmental impacts might increase due to persistent and highly toxic substances that do not belong to the PBT or vPvB categories, or because of the climate change. The amounts in the environment might increase to a level where the adverse effects can be observed. Under these conditions, the success of the substitution is arguable. As an example, a recent study linking the 10 to 60-fold decrease in insect populations over the past 30 years thus impacting the whole food chain in Puerto Rico to greenhouse gas emissions is as alarming as the historical dichlorodiphenyltrichloroethane (DDT) (Lister, Garcia, 2018).

The situation becomes even more dire when we recognize the fact that the regional improvements that have been documented by some studies over the last decades are partly due to the shift of burden to other regions of the world, namely, the ‘3rd world’ countries (Castleman, 2016; Baughen, 1995; Ives, 1985; Shue, 1981). This fact necessitates a life cycle approach in assessing the environmental impacts of alternatives.

Even when an alternative has been determined as a substitute to these problematic substances, regrettable substitution is another concern, such as in the case of brominated flame retardants (BFRs) (Gramatica, Cassani and Sangion, 2016; Zimmerman, Anastas, 2015).

The use of hazardous substances, e.g., in plastics (Hahladakis *et al*., 2018), also hinders circular economy (Bodar *et al*., 2018) thus contributing to the waste problem, such as plastics in the environment.

1.3. Accidental and fugitive emissions

Globally, over a million metric tons of industrial emissions per year stems from fugitive emissions. In the USA alone, it is estimated that fugitive emissions from industry add up to more than 300,000 tons per year, which is about 33% of the total organic chemical emissions from chemical plants (Hassim *et al*., 2012). The situation is similar in the EU. What concerns occupational safety, fatalities from exposure to fugitive emissions exceed those from fatalities due to physical accidents. This is especially the case for the fugitive emissions of carcinogenic substances, even in small amounts, over prolonged periods of time (Hassim *et al*., 2012). It was estimated that, in the EU-27 region, exposure to hazardous substances causes 74,000 worker deaths each year (ILO, 2005).

In the EU-28 region, the manufacturing industry reported that 4.4% of fatal worker accidents were caused by accidental emissions in 2016. These accidental emissions have been reported under categories of overflow, overturn, leak, flow, vaporization and emission (Eurostat, 2016).

1.4. Production amounts of hazardous substances

In 2017, 292 million tons of chemical substances were produced, and 308 million tons of chemical substances were used within the EU-28 region. In the same region during the last 10 years, the production amount of hazardous substances has not changed significantly (except for a slight temporary decrease due to the economic recession of 2008), with approximately 75% of the produced substances being hazardous to human health, with 12% of the produced substances having carcinogenic, mutagenic and reprotoxic (CMR) properties on humans, and with 28% being hazardous to the environment (Eurostat, 2018a). Currently, with a population of 513 million living in the EU-28 region (Eurostat, 2018b), the amount of substances hazardous to human health that is being produced in the EU-28 region is 427 kg per person per year. It can be said that the EU-28 region is producing hazardous substances at a rate equivalent to the minimum drinking water needs of its population. For each glass of water that we drink, we are producing almost that much of hazardous substance.

The consumption of hazardous substances (especially with environmental hazards) is decreasing in the EU-region, although the production rates have not varied much in the last decade (Eurostat, 2018a). The reductions have occurred, especially for CMR and substances that possess a severe chronic environmental hazard, predominantly after the year 2014. Consumption of chemicals with a severe chronic environmental hazard decreased from approximately 8% (average values of 2004–2014) to 2.8% of the total consumption in 2017. For the same time period, the consumption of CMR substances was reduced from 12.4% to 9.3%, and once again the reductions were predominantly observed after 2014 (Eurostat, 2018a). These reductions are highlighted to be driven primarily by strict restriction and authorization requirements for some SVHC under REACH regulation, rather than by company decisions based on chemical alternatives assessment frameworks. According to the Eurostat database, the constant production amounts and the decreasing consumption of SVHC in EU means that hazardous substances are being exported rather than eliminated (Eurostat, 2018a). This fact, once again, highlights the importance of life cycle thinking in terms of not shifting the burden to other countries.

1.5. Review of life cycle impact assessment methods

LCA is a well-established methodology for assessing the environmental impacts of life cycle emissions and resource extraction on ecosystems, humans and resources. Among the three types of LCA (Full (or Complete) LCA, Simplified LCA, Streamlined LCA), Simplified LCA is moderate in terms of the degree of being generic for life cycle inventory (LCI) (EeBGuide Project, 2012). Streamlined LCA (also called *Screening LCA*) is the simplest LCA type that does not require detailed knowledge about the processes in the target company and can be conducted by knowing the product type by using generic LCIs. On the other hand, Simplified LCA uses company specific data obtained from Material Flow Analysis (MFA), and uses generic LCI for the rest of the life cycle.

Life cycle impact assessment (LCIA) methods are under constant improvement. As the science progresses, the modelling approaches and the scope of impacts as well as the regional differences are incorporated into these methodologies. Although methods based on policy targets do exist, methods that are based on the cause-effect chain modelling are considered to be more scientifically sound (Rosenbaum, 2018).

A number of methods used for 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, etc.), while other methods employ impact category indicators at the endpoint level (such as damage to human health and damage to the ecosystem quality).

The aim of the LCA indicators is to provide quantitative information on the extent to which the negative impact to the environment, human health and resources has been reduced due to the substitution of hazardous chemicals. Impact can be reduced for three Areas of Protection (AoP): environment, human health and resources. AoP simply means the entities that need to be protected – such as humans, freshwater organisms, etc.

In LCA, characterization factors are values specific to each condition (e.g., substance, impact category, etc.) that, when multiplied with the emissions, give the impacts of the corresponding impact category. 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 midpoint impact categories, a normalization step should be implemented. Normalization is done by normalizing the environmental impact of the product to the environmental impact of the average EU citizen for each midpoint impact category. Although normalization should preferably be based on the carrying capacity of the ecosystem, currently, this approach is still under development (Bjørn, Hauschild, 2015). For endpoint impact scores, instead of applying normalization, the midpoint impact scores are used to calculate the direct impacts on AoP (Huijbregts *et al.*, 2016). Although endpoint impact indicators are denoted by higher uncertainty than midpoint impact indicators, endpoint impact indicators are easier to interpret, and they are more convenient to use with other methods evaluating harm to the AoP.

The most recent and widely used LCIA methods have been considered for review according to their suitability to be used in this thesis due to the fact that the latest methods are the improved versions of the older methods. The endpoint impact assessment methods which calculate direct harm on the AoP rather than the quantification of the harming agent are easier to interpret for inexpert assessors. As one of the aims of this thesis is to also target SMEs, the LCIA methods that integrate endpoint impact categories have been considered as well. Also, the case studies available for this thesis were within the EU region, hence regional considerations of the suitable LCIA method should be Europe-oriented.

The most commonly used LCIA methods are (Rosenbaum, 2018; European Union [EU], 2010b): EDIP (Hauschild and Wenzel, 1998), EPS (Steen, 1999), Eco-indicator 99 (Goedkoop and Spriensma, 2000), CML (Guinée *et al*., 2002), IMPACT 2002+ (Jolliet *et al*., 2003), LUCAS of Canada (Toffoletto *et al*., 2007), ReCiPe 2008 (Goedkoop *et al*., 2009), TRACI (Bare, 2011), and LIME 2.0 of Japan (Itsubo and Inaba, 2012). Except for TRACI and LINE 2.0, these methods have been developed by modelling the region of Western Europe.

The latest update to ReCiPe method is ReCiPe 2016 (Huijbregts *et al*., 2016). ReCiPe 2016 builds on ReCiPe 2008 methodology by adding the impact of water use on human health, water use and climate change on freshwater ecosystems, and water use and tropospheric ozone formation on terrestrial ecosystems (Huijbregts *et al*., 2016). Also, some impact categories have been improved by modelling at a global scale, while also maintaining the country/continent specific modelling for impacts that need more local modelling.

Another recent improvement is IMPACT World+ which updates the IMPACT 2002+ method (Rosenbaum, 2018). IMPACT World+, as ReCiPe 2016, also considers impacts at different regional scales, such as global, continental and country scales. Some novel impacts are water consumption impacts on human health, the long-term impacts of marine acidification on the ecosystem quality, and the thermally polluted river water.

1.6. Review of the chemical alternatives assessment frameworks

A variety of supplementary frameworks have been developed to aid substitution. As an example, in 2006 ‘Alternatives Assessment Framework of the Lowell Center for Sustainable Production’ was published as a guide for alternatives assessment stating its purpose as “Creating an open source framework for the relatively quick assessment of safer and more socially just alternatives to chemicals, materials, and products of concern. ‘Open source’ in this context means the collaborative development, sharing, and growth of methods, tools, and databases that facilitate decision making. ‘Relatively quick assessment’ presently means that the process results in robust decisions informed by the best available science, while avoiding paralysis by analysis” (Rossi, Tickner and Geiser, 2006). In the same year, assessment was conducted by the Massachusetts Toxics Use Reduction Institute of University of Massachusetts Lowell, known as the ‘Five Chemicals Alternatives Assessment Study’, which successfully identified alternatives for the selected substances of concern (Eliason, Morose, 2011).

There are a number of frameworks targeting this issue, and their scope and methodology spread over a large domain. Frameworks are usually designed to be implemented by regulatory bodies as well as other assessors with various resource capabilities. Voluntary alternatives assessments performed by non-regulatory bodies for various purposes (e.g., company policy, advertisement, technological improvement, etc.) other than regulatory restrictions should be widespread and well-established. The number of voluntary substitutions in companies might be seen as an indicator of the technological process development. Nevertheless, alternatives assessments should be available to most companies for the sake of minimizing the chance of regrettable substitution.

As in any assessment, the available time, available resources and the state of the assessment methodology are the limiting factors. Improvement of the assessment can be accomplished by the improvement of these three variables. Hence, the successful framework should present a methodology which is sufficiently established to enable most of the companies to perform a comprehensive assessment by increasing their efficiency of using the available resources and the available time, or else by presenting easier-to-use and automated assessments. Here, ‘comprehensive’ means the most recent state-of-the-art pathways for the protection of the humans, the environment and the resources. However, ‘comprehensive’ does not necessarily mean more complex or hard to implement.

This becomes very important as SMEs are a major part of the global production (Hussey, Eagan, 2007), and the regulatory requirements are set only for the major issues while ignoring the fact that the aggregation of many small impacts leads to a big impact. Some of the ‘small issues’ that regulatory requirements mostly exclude are the releases other than the release of CMR, persistent, bio-accumulative and toxic (PBT), or very persistent and very bio-accumulative (vPvB) substances throughout a product’s life cycle, including the transportation and waste treatment stage. As the SMEs are a major part of the global production, they can vastly contribute to the environmental impacts. At the same time, they have limited resources that hinder the comprehensive environmental impact assessment process; hence, it is important to focus on SMEs in order to reduce the negative environmental impact of the technological production processes. Today, companies in most cases do not have the tools to choose their inputs based on the comprehensive environmental impact of their choices. A materials safety data sheet (MSDS) that shows human health hazards, environmental hazards, and the cost of the product is what they only have, yet without the relevant information about the life cycle impacts of those products. There is a lot of room for improvement; and, for this purpose, six frameworks have been chosen and reviewed for specific features without being exhaustive so that to determine the state-of-the-art requirements in chemicals substitution and assessments regarding environmental protection.

The six selected frameworks are as follows: National Academy of Sciences (NAS) (NRC, 2014), Interstate Chemicals Clearinghouse (IC2, 2013), German Guide on Sustainable Chemicals (Reihlen *et al*., 2011), Biz-NGO (Rossi, Peele and Thorpe, 2011), Ontario Toxics Use Reduction Program (Ontario Toxics Use Reduction Program, 2012) and Lowell Center for Sustainable Production (Rossi *et al*., 2006). The selected frameworks are based on the following criteria: they must be published after 2005 the frameworks are selected to be representative of the latest progress for their publication year that might be from 2006 to 2016, they must be tailored for the substitution of hazardous chemicals in general, must include the implementation of a life cycle assessment (LCA) and must be suitable for assessors with limited resources (e.g., SMEs). Frameworks that incorporate LCA have been prioritized. Information for the selection criteria of the major frameworks can be seen in Table 1.1.

Table 1.1. General information on major frameworks

		Selection Criteria		
Name	**Country of origin**	**Suggests LCA in main framework**	**Other information**	**The selected frameworks for the review**
National Academy of Sciences (NRC, 2014)	USA	✓	A unified, multi-purpose* alternatives assessment framework by the review of predecessor frameworks	✓
Interstate Chemicals Clearinghouse (IC2, 2013)	USA	✓	A multi-purpose* alternatives assessment framework	✓
German Guide on Sustainable Chemicals (Reihlen *et al*., 2011)	Germany		Developed particularly to guide SMEs in the selection of sustainable chemicals	✓
Biz-NGO (Rossi *et al*., 2011)	USA	✓	A multi-purpose* alternatives assessment framework	✓
Ontario Toxics Use Reduction Program (Ontario Toxics Use Reduction Program, 2012)	Canada	✓	A unified, multi-purpose* alternatives assessment framework by the review of predecessor frameworks	✓
Lowell (Rossi *et al*., 2006)	USA	✓	A multi-purpose* alternatives assessment framework	✓
US OSHA (US OSHA, 2013)	USA		Developed to address work place safety	
European Commission, DGE (EC DGE, 2012)	Europe		Developed to address work place safety	
US EPA SNAP Program (US EPA, 2011b)	USA		A framework for particular sectors	
REACH (ECHA, 2011)	Europe		Developed as a regulatory support for substitution of hazardous chemicals	
UCLA Sustainable Policy & Technology Program (Malloy *et al*., 2011; Malloy *et al*., 2013)	USA		A regulatory alternatives assessment framework	
US EPA DFE Program (Lavoie et *al*., 2010; US EPA, 2011a)	USA		An alternatives assessment framework that involves regulatory bodies	
UNEP (UNEP, 2009)	International		Developed for the substitution of Persistent Organic Pollutants (POPs)	
TRGS 600 (BauA, 2008)	Germany		Developed as regulatory support for work place safety	
P2OSH (Quinn *et al*., 2006)	USA		Sector specific framework	

		Selection Criteria		
Name	**Country of origin**	**Suggests LCA in main framework**	**Other information**	**The selected frameworks for the review**
MA TURI (MA TURI, 2006; Eliason, Morose, 2011)	USA		A multi-purpose* alternatives assessment framework	
Rosenberg *et al*. (2001)	USA		Developed to address work place safety	
US EPA CTSA (US EPA, 1996)	USA		An alternatives assessment framework that involves regulatory bodies	
Goldschmidt (Goldschmidt, 1993)	Denmark		Developed to address work place safety	

***** *Here, multi-purpose means that it can be used by assessors with a variety of resource availability so that to conduct an alternatives assessment of chemicals in various industries.*

The purpose of this review is to stress the resource limitation problems in the current frameworks, to review the employed assessments and to consider how the assessments are being used in combination, to point out the future development possibilities of the alternatives assessment frameworks for the implementation in SMEs and other assessors with more resources, and to stress the possibilities of modifying the encountered tools and assessments so that to render them suitable for life cycle thinking to be used in the environmental impact assessment model of this thesis. A more comprehensive review covering other aspects of chemicals alternatives assessment frameworks can be found in the work of Molly M. Jacobs, Timothy F. Malloy, Joel A. Tickner, and Sally Edwards (Jacobs *et al*., 2016).

1.6.1.Methodology for reviewing the chemical alternatives assessment frameworks

The frameworks are a combination of various assessments (e.g., hazard assessment) that evaluate the important aspects of substitution. Each of the frameworks has been examined for the following features: assessments included, assessment flowchart structure, inclusion of SMEs in terms of resource intensity, tools and methods included or guided to, and indicators. Assessments, tools and methods, and the flowchart structure have been included because they are important in resource management and may affect the outcome of the alternatives assessment. The differences among the methods/tools can be the extent of the scope (i.e., inclusion of the necessary criteria), or the use of different approaches. The methods referred in the frameworks as easy to implement do usually exclude certain aspects which could render the assessment easier. It is the same with the use of the elimination methods. Sequential elimination methods are used when the framework targets to make the overall alternatives assessment easier for the SMEs. Inclusion of SMEs has been reviewed because of the importance of voluntary substitution and the fact that SMEs are a major part of the global production (Hussey, Eagan, 2007). Indicators have been reviewed in order to find a set of potential practical indicators to be used at the follow up stage after the implementation of the alternatives assessment. The main sources that frameworks guide to (such as the tools and methods) are also included and have been seen as a whole with the framework which it is included in, whenever the framework uses them as a basic tool/method or optionally guides to them. One main problem is that although the frameworks which optionally guide to more than one method/tool can be seen comprehensive in one aspect, it should be noted that assessors have the freedom to select a few of those methods/tools. During the review, the frameworks will be evaluated with their ‘total scope’ (i.e., including the assessments that frameworks refer to) without being exhaustive, and notes will be added if necessary. The assessments have been regarded as mandatory if they are not mentioned as optional in the frameworks.

For the purpose of this review, the main assessments observed are grouped as: Physicochemical, Human health hazard, Exposure, Environmental, Technical performance, Economic/Financial, Social and Life Cycle Assessment (LCA). In the present review, physicochemical assessment is any assessment that uses physicochemical properties of the chemicals to evaluate physicochemical hazards (e.g., explosive, corrosive, etc.) and/or to further predict the properties of the chemicals to be used in subsequent assessment(s). During the thesis, the definition of physicochemical properties will be the same as NAS framework's definition: "[...] physicochemical properties are broadly defined as physical properties, solvation properties related to interactions with different media and properties or molecular attributes that define intrinsic chemical reactivity" (NRC, 2014). Human health hazard assessment evaluates the intrinsic hazards of the chemicals to humans other than the physicochemical hazards. Exposure assessment is used as the means of any assessment that includes exposure models or simply uses physicochemical properties to evaluate exposure potential without any modelling to any AoP. Environmental assessment takes into account the intrinsic hazards of the chemicals to the environment, such as ecotoxicity hazards. Technical performance assessment examines the alternative's technical performance for a required function. Economic/Financial and social assessment evaluates the economic/financial and social aspects of the substitution, respectively, and might include life cycle thinking. Life cycle assessment (LCA) evaluates the life cycle impacts of the alternative and the chemical of concern on the environment and humans.

It has been observed, however, that, in some cases, those assessments are strongly linked to each other, and it is thus not possible to draw a strict line between them. For example, in some frameworks, physicochemical properties may also be used to predict the toxicity of the substance, hence, they can be seen as a part of the human health hazard assessment. Some frameworks may guide to a comprehensive exposure assessment, while others (e.g., Lowell) may use only a few criteria (e.g., vapor pressure) to address the exposure potential. Hence, those connections have been noted in this thesis; even when the assessment names are the same, the details and scope might differ for each framework.

Finally, the known case studies are critically reviewed in Section 1.6.7 with the information from the previous sections of this review.

1.6.2.Assessments included

It is important to have an idea on the major methods that frameworks often refer to before continuing with the review. In the following Section, some major methods/tools are presented.

The GreenScreen® method (Clean Production Action [CPA], 2013) is a semi-quantitative and comparative hazard assessment method that addresses environmental and human health impacts. Qualitative information, such as 'eye irritation', as well as quantitative data such as 'toxicity' is used as a hazard criterion. The method is based on the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) (UN, 2011) hazard criteria and takes into account the degradation products that can be a concern. The substance of concern and the alternative substances are classified in five categories (i.e., benchmarks) depending on the hazards of the chemicals; the uncertainty of the data on chemicals is also taken into account. The evaluation of uncertainty is qualitative and might need expert judgement. In the case of missing data about the critical features of the chemical (defined by the method), the chemical is noted as *Benchmark U* (i.e., unspecified chemical hazard). The hazard categories include CMR, developmental toxicity, endocrine activity, acute mammalian toxicity, systemic organ toxicity (STOT), neurotoxicity, skin sensitization, respiratory sensitization, skin irritation and corrosivity, eye irritation and corrosivity, acute aquatic toxicity, chronic aquatic toxicity, reactivity, flammability, persistence, bioaccumulation and other ecotoxicity studies if available. Despite the availability of this accomplished chemical hazard assessment tool, the procedure of the method can be quite complex for inexpert assessors, hence it is not suitable for SMEs (Subsport, 2016a; Edwards *et al*., 2011).

The GreenScreen List Translator is a consolidation of regulatory and scientific lists on hazards to be used in the GreenScreen method. The list translator can also be used as the indicator of chemicals of high concern (CPA, 2013).

The Column Model (IFA, 2017) is similar to the GreenScreen® method but it is easier to implement. The hazard data is obtained from the material safety data sheets (MSDS) and used to classify chemicals under six categories and assign each chemical a note (e.g., very high risk, high risk, medium risk, etc.) for each category according to their chemical hazards. The missing data is assigned to different risk categories depending on the type of the missing data. The decision is made by the assessor based on their judgement and knowledge about the use patterns and use amounts of the chemical.

The Quick Scan (Dutch Ministry of Housing, 2002) is a semi-quantitative method that assigns categories to chemicals based on their hazards (e.g., high concern, etc.) as well as exposure potential (e.g., high exposure, etc.). The exposure potential is based on the use type of the chemical (e.g., open professional use, site limited intermediate substances, etc.). The tool can be seen as a very simplified risk assessment strategy. Any missing data leads to a material being assigned to high risk. The tool was developed after the discussions at the Dutch Ministry of Housing, Spatial Planning and the Environment in 2001, and it was agreed that additional support should be given to SMEs by developing easy to-use-tools for the substitution of hazardous substances (Dutch Ministry of Housing, 2002). According to the Subsport substitution portal, this effort to make the assessment easy enough for the implementation by SMEs has not been successful (Subsport, 2016b).

QCAT (Washington State Department of Ecology, 2015) is based on the GreenScreen® method, but it excludes physical hazards and some part of human health and ecological hazards in order to simplify the assessment. The hazard categories include CMR, developmental toxicity, endocrine activity, acute mammalian toxicity, acute aquatic toxicity, persistence, and bioaccumulation. This simplification in return increases the risks of a regrettable substitution whenever the tool is utilized (Washington State Department of Ecology, 2015).

The ECETOC TRA risk assessment tool (European Centre for Ecotoxicology and Toxicology of Chemicals [ECETOC], 2014) is a quantitative, exposure model-based tool that assesses risks to workers, consumers and the environment.

The PRIO tool (KemI, 2015) evaluates chemicals of concern under two categories: the phase-out substances, and the priority risk-reduction substances. The phase-out substances include CMR, PBT, vPvB, particularly hazardous metals, endocrine disruptive substances, and ozone-depleting substances. The priority risk-reduction substances include very high acute toxicity, allergenic, mutagenic (category 2), high chronic toxicity, ozone depletion potential, aquatic toxicity, and potential PBT or vPvB substances. It is also possible to evaluate risks based on the use patterns, similarly to QCAT. The tool is also semi-qualitative.

The TURI Pollution Prevention Options Analysis System (P2OASys) (Toxics Use Reduction Institute [TURI], 2015; Edwards *et al.*, 2011) is a comparative hazard and exposure assessment tool intended to evaluate the impacts of chemicals on the environment and workers. Exposure can be evaluated by use patterns, and uncertainties are subsequently addressed. The tool is not publicly available.

Life Cycle Assessment (LCA) is a quantitative method developed for comparative evaluation of products based on the environmental impacts (climate change, ozone depletion, terrestrial acidification, freshwater eutrophication, marine eutrophication, human toxicity, photochemical oxidant formation, particulate matter formation, terrestrial ecotoxicity, freshwater ecotoxicity, marine ecotoxicity, ionising radiation, agricultural land occupation, urban land occupation, natural land transformation, water depletion, mineral resource depletion, fossil fuel depletion, etc.) of the input-outputs of the entire life cycle of each product; “from cradle to grave” (EU, 2010b). Each impact category used in the LCA study is described in quantitative units. Modelling of the system to be examined is being done by multiple approaches (e.g., the consequential modelling approach, the attributional modelling approach, etc.) to be used for different purposes so that it could yield different results from each other (United Nations Environment Program [UNEP], 2011). The consequential modelling approach is more convenient if changes to the technosphere are detected, as in the case of alternatives assessment.

More detailed information on the analysis of some of these methods/tools can be obtained from the work by Sally Edwards, Joel Tickner, Yve Torrie, Melissa Coffin and Laura Kernan (Edwards *et al.*, 2011). Jacobs *et al*. states: “[...] the need for a more streamlined approach to identifying life-cycle impacts. However, greater methodological clarity about what is encompassed in life-cycle thinking would be of benefit to the alternatives assessment field” (Jacobs *et al.*, 2016).

Physicochemical assessment

Physicochemical properties are assessed to a different extent among the frameworks. NAS and IC2 frameworks use physicochemical properties (such as vapor pressure, solubility, boiling/melting point, etc.) to further predict the exposure potential and also as the initial elimination criteria. The German Guide also uses physicochemical properties under the name ‘mobility’ criteria (such as solubility in water, vapor pressure, etc.) to evaluate the exposure potential. Biz-NGO and Lowell frameworks use physicochemical properties to a limited extent. While the German Guide takes into account the explosive, oxidizing, flammability and pyrophoric properties for hazard assessment, Biz-NGO and the Ontario Toxics Use Reduction Program address this by guiding to the GreenScreen® method (CPA, 2013) which assesses reactivity and flammability, and Lowell framework by directing to many other methods (such as the Column Model, the Quick Scan, etc.) which assess the flammability, explosive properties and vapor pressure, etc. If the assessor selects to implement the Column Model, then flammability, explosion, oxidizing, pyrophoric and corrosivity hazards are being assessed, while vapor pressure is used to evaluate the exposure potential. The Ontario Toxics Use Reduction Program also uses physicochemical information (i.e., corrosivity, reactivity, flammability and vapor pressure) to assess occupational health and safety as well as some other physicochemical properties in its technical feasibility assessment.

Human health hazard assessment

Human health hazard assessments are mandatory and included in all the frameworks to a similar extent; the hazard criteria are defined within the frameworks or by guidance to tools/methods and authoritative lists, usually in parallel with the Design for the Environment (DfE) hazard criteria (United States Environmental Protection Agency [US EPA], 2011a) and CLP hazard criteria. The *Globally Harmonized System of Classification and Labelling of Chemicals* (UN, 2011) is frequently used in the frameworks as a hazard indicator. The IC2 framework also has an optional initial screening step for hazard evaluation. *Ontario Toxics Use Reduction Program* has a mandatory preliminary assessment that uses regulatory lists which take into account CMR, PBT, vPvB properties and other hazards that are critical to today’s environment and human well-being, and also takes into account the degradation products (Ontario Toxics Use Reduction Program, 2012). In the IC2 framework, this preliminary assessment is optional. The Lowell framework also refers to the PRIO tool. All frameworks take into account the impact of the degradation products by implementing the GreenScreen® method (CPA, 2013).

Exposure assessment

In the frameworks, exposure can be assessed for humans, environmental compartments, consumers or workers and for different stages, such as use and disposal. This separation has been made in order to consider various AoP and to be able to focus on the most relevant impacts. All frameworks include exposure considerations to some extent (i.e., by exposure models, or only by assessing physicochemical properties, such as vapor pressure, etc.). As the NAS framework mentions, data on the exposure can be obtained from exposure models or from physicochemical properties as mentioned above (NRC, 2014). Biodegradation and bioaccumulation are examples of features that affect exposure and can be derived from physicochemical properties (NRC, 2014). In the NAS framework, those predictions derived by using physicochemical properties are then employed to define the scope of further assessments. For example, if a chemical is denoted by high water solubility, then the focus of exposure assessment will be the aquatic environments. The IC2 framework has an initial screening assessment within the exposure module which determines whether the alternative(s) and the chemical of concern are similar enough to show similar exposure potential, so that any further exposure assessment can be omitted. The Biz-NGO framework suggests that hazard assessments might be sufficient for the alternatives assessment, and it might not be necessary to conduct an exposure assessment for all alternatives as this framework assumes that the most effective way of reducing risk is the reduction of hazard. The *Ontario Toxics Use Reduction Program* sets exposure limits for workers. The Lowell framework refers to the 'Column model' which uses vapor pressure to predict the exposure potential. The *German Guide* framework refers to the *ECETOC TRA* tool (ECETOC, 2014) for the quantitative evaluation of worker, human and environmental exposure, but also uses physicochemical properties to predict the exposure potential.

Environmental assessment

Environmental assessment is in the scope of all frameworks. DfE (US EPA, 2011a) hazard criteria usually form the basis for this assessment. Those criteria include persistence, bioaccumulation, and acute as well as chronic aquatic toxicity. Some frameworks, such as IC2, include other criteria (e.g., eutrophication potential, phytotoxicity). The Lowell framework guides to the PRIO hazard assessment tool that considers ozone depletion and aquatic toxicity in its hazard assessment section (KemI, 2015), whereas the NAS framework assesses sediment and terrestrial toxicity as well. Any criteria other than DfEs are rarely assessed for environmental impacts in other frameworks. Frameworks usually use authoritative lists for preliminary evaluation. All frameworks take into account the impact of degradation products by implementing the GreenScreen® method.

Technical performance assessment

Technical performance issues for products are addressed in all frameworks. Most frameworks mention the use of already existing (well proven) technologies, which, if possible, would decrease the need for this assessment. Biz-NGO notes that the functional approach is important in evaluating the technical performance, and the alternatives should not be compared and assessed with the existing chemical of concern; instead, they must be evaluated in terms of the minimum necessary (required) function that they need to perform in the product/process. As well as the IC2 framework, many frameworks suggest performing assessments parallel with this approach. The NAS framework and the *Ontario Toxics Use Reduction Program* clearly define this assessment as 'optional', and the IC2 framework clearly defines it as 'mandatory' up to the lowest level of the performance evaluation module (the IC2 framework also has an initial screening step for performance as an optional feature).

Economic and Financial assessments

Economic/financial issues are addressed in all frameworks to a different extent. Usually, economic assessments should consider the life cycle of the product, but it is possible to only implement financial assessment and evaluate the cost of the alternative chemical in some frameworks (e.g., economic assessment is mandatory as financial assessment in the IC2 framework only for the alternative chemical(s) and the chemical of concern). The Lowell framework advises not to focus solely on the short-term costs of the substitution. The NAS framework clearly defines this assessment as ‘optional’, whereas the IC2 framework clearly defines it as ‘mandatory’ up to the lowest level of the cost and availability module. In the IC2 framework, Life Cycle Costing (LCC) and Cost Benefit Analysis (CBA) can be conducted at advanced levels. CBA is also implemented in the *Ontario Toxics Use Reduction Program* within the financial evaluation and other assessments that take into account the disposal costs, training costs, etc.

Social assessments

Among the frameworks, only Biz-NGO does not mention the social impacts, nor does it give any reason why the social impacts are not included. The NAS framework suggests some social impact categories for the assessor as guidance, and takes the *Life Cycle Thinking* (LCT) approach. The IC2, the German Guide, the Ontario Toxics Use Reduction Program and the Lowell frameworks also address this issue with life cycle thinking. As an example, the IC2 framework suggests considering social impacts on workers and on the public during the extraction, manufacture, transport, use and disposal stages. The IC2 framework also mentions *Social Life Cycle Assessment* (SLCA) at advanced levels.

Life Cycle Thinking

The NAS framework proposes implementation of a qualitative LCT to identify any differences that might necessitate an LCA; streamlined LCA methods that use averaged data for industrial processes (USEtox (Rosenbaum *et al*., 2011; UNEP SETAC, 2016; USEtox, 2017) fate-exposure-effect model might be used to predict case specific characterization factors, but it is noted that this method is not sufficiently developed yet) might be used if the resources are limited instead of case specific values. The NAS framework also introduces the ‘Synthetic history’ concept which considers the parent chemicals of the alternative chemical and those of the chemical of concern in order to spot any differences that may arise from substitution. Together with the material and energy flow differences, those differences, if any, might justify further LCAs. The IC2 framework, at the initial stage, assesses social, economic and sustainability issues related to raw material usage and waste generation. If any sufficient differences exist between the alternatives themselves and the chemical of concern, it may be justified for the assessor to progress to the higher steps of the framework which include implementation of Material Flow Analysis (MFA) and LCA. The Biz-NGO framework does not justify LCA for human health hazards and environmental toxicity if the alternatives have the same functional use and a similar life cycle; the assumption used in these frameworks is as follows: the exposure results will be similar; hence the hazard assessment can be considered sufficient. The *Ontario Toxics Use Reduction Program* includes a detailed guide to LCA for large companies. The Lowell framework, while finding LCA to be a well-accomplished method, discusses the shortcomings of LCA in certain areas, such as the scope definition, lack of transparency, narrow (pollutant-focused) hazard assessment, insufficient incorporation of the recycling stage, and high costs. In all the frameworks that incorporate LCA, it is defined as 'optional', and its implementation depends on the outcomes of previous assessments and on the resources of the assessor.

A summary of the main features of the frameworks can be found in Table 1.2 and Table 1.3.

Table 1.2. Assessments included in the selected frameworks (not exhaustive)

Assessment		**NAS**	**IC2**	**German Guide**	**Biz-NGO**	**Ontario**	**Lowell**
Physicochemical		✓[1,2]	✓[1,2]°	✓[1,2]	✓[2]	✓[1]°	✓[1,2]
Human health hazard		✓*	✓*	✓*	✓*	✓*	✓*
Exposure	**Worker**	✓*	✓[3]*	✓[6]*	✓[3]*	✓°*	✓[4]*
	Human	✓[5]*	✓[3,5]*	✓[5]*	✓[3,5]*	✓[5]°*	✓[5]*
	Environment	✓[5]*	✓[3,5]*	✓[5]*	✓[3,5]*	✓[5]°*	✓[5]*
Environmental Hazard		✓*	✓*	✓*	✓*	✓*	✓*
Performance		✓°	✓	✓	✓	✓	✓
Economic		✓°*	✓*	✓	✓*	✓*	✓*
Financial		✓°	✓	✓	✓	✓	✓
Social		✓*	✓°*	✓*		✓°*	✓*
LCA		✓°*	✓°*	✓°*	✓°*	✓°*	✓°*

✓ Included/mentioned

° Optional assessments

* Considered in LCT

[1] Physicochemical properties are used indirectly to predict other properties of the substance, such as environmental fate and exposure.

[2] Physicochemical properties are directly used to eliminate such alternatives as the initial screening.

[3] Optional only if there is no necessity determined by previous assessments within the framework.

[4] Only physicochemical properties are used to evaluate exposure

[5] Exposure models used to evaluate the exposure at advanced levels (LCA incorporates exposure models)

[6] Exposure models used to evaluate the exposure in advanced levels (ECETOC TRA)

Table 1.3. Basic features adopted in the selected frameworks

	NAS	IC2	German Guide	Biz-NGO	Ontario	Lowell
Elimination method	Hybrid	Any	Hybrid	Hybrid	Hybrid	Any
Decision tools/methods	✓ (MCDA and other)	✓	✓ (Golden rules)	✓ (CPA, 2013)	✓ (Green Chemistry Principles and MCDA)	✓
Product/Process Change	✓	✓	✓	✓	✓	✓
Data gaps	✓	✓	✓	✓ (CPA, 2013)	✓ (CPA, 2013)	✓
LCT	✓	✓	✓	✓	✓	✓

✓ Mentioned

1.6.3. Flowchart structure

Almost all frameworks demonstrate a gradual approach towards the implementation of assessments, starting from basic and easy-to-implement aspects and moving towards more comprehensive assessments with an increasing difficulty. The minimum level of assessments to avoid regrettable substitution is defined in most frameworks.

The NAS framework adopts a hybrid elimination approach which is a combination of simultaneous and sequential elimination methods. The difference between the simultaneous and sequential elimination method is that the selection of alternative(s) to be carried to the next step of the framework is decided upon simultaneously, by weighting, while the selection of alternative(s) to be carried to the next step of the framework is decided by one assessment at a time (hence the outcome depends on the assessment flowchart order), respectively. If both elimination methods are used in combination, it is called a hybrid elimination method. The IC2 framework is divided into modules which are further divided into levels (comprising questions) depending on the difficulty and comprehensiveness of tasks. Besides, the framework can be implemented in a hybrid, simultaneous or sequential form depending on the assessor’s capabilities. In the German Guide, this is not clearly defined. The German Guide is a hybrid in the sense that substance specific and use specific assessments are implemented sequentially, and within each of those two sections, the framework can be simultaneous or sequential as well. Biz-NGO is a hybrid framework, but it is heavily sequential rather than simultaneous. The *Ontario Toxics Use Reduction Program* adopts a preliminary elimination approach; thus the framework structure is hybrid. The Lowell framework’s structure is based on the ‘Guiding principles’ that are determined by the assessor, hence it can be hybrid, simultaneous, or sequential.

1.6.4. Inclusion of SME’s

The NAS framework is designed for different assessors with different resource capabilities. The framework has mandatory assessments (at a minimum, the NAS committee recommends the implementation of physicochemical, exposure, ecotoxicity, human health hazard assessments and life cycle thinking) to be conducted so that to prevent regrettable substitution as much as possible. Assessors might consider to further assess broader environmental impacts (e.g., resource use, climate change) if they are relevant. Throughout the framework, the purpose of databases and tools is clearly defined. The use of physicochemical properties to simplify the subsequent assessments (e.g., exposure, etc.) is well-established. Decision methods are also mentioned (e.g., *Multi-criteria Decision Analysis* (MCDA)). Data gaps are handled with different methods (e.g., the *in vitro* and *in silico* methods), but most of them are advanced and need expertise (NRC, 2014). The IC2 framework notes that the GreenScreen® method might be difficult for inexpert assessors to implement, and guides to simpler tools such as 'list translators' (e.g., the GreenScreen® List Translator), and the *Quick Chemical Assessment Tool* (QCAT) with a warning about the regrettable substitution potential in case of using those simplified tools. The IC2 framework is divided into modules for each assessment which then are subsequently divided into levels in terms of difficulty and comprehensiveness. It is formed of a questionnaire in the flowchart structure and also guides to tools and databases whenever necessary. Decision methods are mentioned, and uncertainties and data gaps are addressed by the GreenScreen® method in the framework. On the other hand, the German Guide is not clear about the decision methods. While data gaps are incorporated in the framework structure, and the German Guide framework is very clear about data gaps, it does not guide the assessor in terms of uncertainties. The Biz-NGO framework's structure is heavily sequential, which may be good for effective resource management, but, on the other hand, there is a higher possibility of overlooking possible alternatives. In addition, the *Quick Chemical Assessment Tool* (QCAT) is mentioned, which is a simplified tool, with a downside of a higher probability of regrettable substitution. Nevertheless, the framework is suitable for SMEs in the resource management aspect thanks to its sequential elimination approach. The *Ontario Toxics Use Reduction Program* recommends the assessors in the same sector to combine their resources in searching for an alternative, and ideally not to work independently. At each step of the framework, the relevance of the step is defined for SMEs and for large companies. The framework references many databases where assessors can search for substitution cases similar to their case. Preliminary technical, financial assessment and evaluation of the presence on regulatory lists are implemented to reduce the number of alternatives to be evaluated at further steps. The major regulatory lists are referenced clearly for this purpose. The subsequent assessments of the framework are optional. The Lowell Center's framework is designed to be flexible in terms of decision rules and guiding principles, and the assessors are free to implement the framework parallel to their own principles. The framework guides to many tools and methods, including decision tools, but some of them (e.g., QuickScan, etc.) are not suitable for assessors without expertise (Subsport, 2016b).

1.6.5. Tools and methods in use

The NAS framework guides to hazard assessment and decision tools, such as GreenScreen® and *UCLA Multi-Criteria Decision Analysis*, respectively. The *Globally Harmonized System of Classification and Labelling of Chemicals* (GHS) (UN, 2011) and authoritative lists are used as the main data source. In addition, the physicochemical properties, high throughput and *Quantitative Structure Activity Relationship* (QSAR) methods (e.g., the *Toxicity Estimation Software Tool* (US EPA, 2016), Ecological Structure-Activity Relationships (US EPA, 2015) (for aquatic toxicity) and OECD QSAR Toolbox (the *Organisation for Economic Co-operation and Development* [OECD], 2016a)) are used for filling in the data gaps. The framework also suggests using the slope of the dose-response curves from toxicity tests as an indication of toxicity risk. The framework includes methods and approaches that use physicochemical properties to predict the environmental fate, persistence, bioavailability of inorganics, as well as the bioaccumulation and toxicity of chemicals. It also guides to ToxPi software (*Carolina Center for Computational Toxicology*, 2010) for visualization of toxicity. The framework guides to standard tests (i.e., Bioassays for aquatic, terrestrial and sediment) for the evaluation of toxicity if the appropriate resources are available. Approaches towards handling uncertainties and trade-offs (e.g., *Multi-Criteria Decision Analysis* (MCDA)) are mentioned in detail, examples to decision rules are given, and it is up to the assessor which one to use among them. At the problem formulation step, the possibility of the process/product change is questioned.

The IC2 framework uses material safety data sheets (MSDS) and authoritative lists in addition to other sources (e.g., the *European Union Substitution Portal*, Innovadex, CleanGredients and 'list translators') as their data source. The *GreenScreen for Hazard Assessment* tool (GreenScreen®) is suggested for hazard assessment. The *Sustainable Materials Management* (OECD, 2016b) approach is used in the materials management module; at the advanced level, *Material Flow Accounting* (MFA) or LCA methods can be used. Decision methods are defined as: the Simple Comparison Method, the Iterative Comparison Method, and the Simultaneous Comparison Method. The IC2 framework also uses Multi-Parameter Analysis as a decision tool. The framework addresses the possibility of process/product change.

The German Guide framework gives advice for substitution as '10 Golden Rules' (e.g., avoid substances mentioned in problematic substance lists, prefer renewable substances, prefer short transport, etc.) as a rule of thumb, and those rules are also used as a qualitative decision method. It also refers to the ECETOC TRA tool (ECETOC, 2014) for quantitative exposure assessment to workers, humans and the environment.

Biz-NGO uses the GreenScreen® tool for hazard assessment. The GreenScreen® tool itself guides to many databases for hazards and deals with decisions regarding data gaps. The framework mentions the *Quantitative Structure Activity Relationship* (QSAR) method suggesting its employment to fill in the data gaps. As a pre-screening tool, the *Quick Chemical Assessment Tool* (QCAT) has been mentioned. It should be noted that QCAT also guides to such databases as ECOTOX. The functionality approach has been adopted which questions the function of the chemical of concern, hence the product/process change is considered.

In the *Ontario Toxics Use Reduction Program*, the Principles of Green Chemistry have been adapted as a general and also as a qualitative selection guide, and the process/product change has been reminded without any description. The GreenScreen® tool for hazard assessment, The *Scoring and Ranking Assessment Model* (SCRAM) (Snyder *et al*., 2000a, b, c and d; Mitchell *et al*., 2002), the *TURI Pollution Prevention Options Analysis System* (P2OASys) (TURI, 2015) are among the sources that are referenced for hazard assessment. In case of data gaps, the framework suggests involvement of experts. For quantitative decision methods, the framework suggests implementation of ranking and weighting methods and references to some examples.

The Lowell framework also defines ‘Guiding Principles’ as the German Guide’s decision rules, but those principles are not strictly defined as in the German Guide, rather, their examples are given (e.g., Prevention, Precaution (Data gaps addressed), Substitution (Process/product change involved), Life Cycle approach, Transparency, Stake holder participation, Continuous improvement, etc.). Besides, for the selection of alternatives, thresholds can be set so that the alternatives with aspects higher/lower than the threshold values would be rejected. Decision methods have also been described (e.g., scoring and weighting). The framework refers to many hazard assessment methods and tools, such as the ‘Column model’ which considers exposure to a limited extent (i.e., uses vapor pressure to predict exposure), PRIO, P2OASys, Quick Scan, GreenList process, Column Model, etc. The Lowell framework also emphasizes thinking about the future as well during the decision making for the selection of alternatives for social, environmental and technical aspects.

Frameworks do not consider error reduction methods. Error propagation studies encountered in the scientific literature focus on various methods for the aggregation of inventories with uncertainties (Heijungs, Lenzen, 2014; Groen *et al*., 2014; Tetreault *et al*., 2013). However, to the best of the author’s knowledge, no studies exist that examine the effects of aggregation of random mistakes made by the assessor on the outcome of the assessment.

1.6.6. Indicators in use

Frameworks usually do not give indicators for the follow-up after the implementation of the substitution. An exception is the NAS framework which guides to bioassays for toxicity that may be used to derive the indicators for toxicity. In addition, the frameworks that use LCA might give an insight on how to select the indicators (e.g., IC2 refers to RECIPE 2008 method, hence indicators). Nevertheless, the assessor must decide which indicator is the most appropriate for their case, and frameworks do not have any direct suggestion on indicators.

1.6.7. Example chemicals alternatives assessment case studies and their relevance to SMEs

The case study “Alternatives to Methylene Chloride in Paint and Varnish Strippers” conducted by Biz-NGO in 2015 (Jacobs, Wang and Rossi, 2015) uses the GreenScreen method to assess chemical hazards. More case studies are expected to be published by Biz-NGO for major hazardous chemicals. It is known that this tool is not suitable for SMEs, hence, the results of the case study conducted by Biz-NGO can only be adapted to SMEs for this specific chemical and usage, and it is not possible for SMEs to apply these case studies to their own specific cases. Additionally, these studies do not address life cycle concerns.

“Chemical substitution of a restricted substance (decaBDE)” and “Chemical Substitution of a Hazardous Biologically Active Compound (Glitazone)” case studies were conducted by the NAS framework in 2014 (NRC, 2014). Both studies use GreenScreen for the hazard assessment step. Both studies are not suitable examples for the SMEs.

No other case studies could be found as a suitable example for the implementation of alternatives assessment including LCA by SMEs.

1.7. Review of life cycle occupational safety methodologies and selection for further review

Risk assessment (RA) is a very broad term used to describe any assessment with a goal of calculating the probability of harm to a valuable entity, usually to humans and to the environment. Harm can be due to many factors, such as chemical emissions and physical accidents. Different types of RA focus on different pathways of harm to different AoP. Usually the results from chemical or radioactivity exposure related quantitative risk assessments (QRAs) are based on the total exposure amount and are used in comparison with a threshold value which determines if the risk is considered as acceptable or not.

The Traditional LCA strictly focuses on chemical emissions and resource depletion, and it evaluates the impacts (either based on solely supply chain/product parts impacts (attributional) or more comprehensive total impacts of options (consequential)) in a comparative manner among the possible options instead of comparing it with a threshold value. LCA cannot be used to evaluate whether the process under examination is safe to an acceptable level or not. The main strength of the LCA methodology is its scope of impacts, such as the climate change, resource depletion, etc., that risk assessments cannot cover due to high uncertainties, and its non-local nature in calculation of these impacts. Nonetheless, location specific life cycle impact assessments (LCIAs) for different impacts are under research (Yang, 2016; Mutel, Hellweg, 2009); the patterns are leading towards narrowing the differences between RA and LCA.

The two methodologies have been accepted to be of high importance in and by themselves, and they cover different scopes. While RA and LCA have important differences, many studies that the author came across in the literature review discuss the compatibility of RA and LCA with each other or attempt to merge these two methods together (Badr *et al*., 2017; Khakzad *et al*., 2017; Eckelman, 2016; Strogen *et al*., 2016; Harder *et al*., 2015; Kobayashi, Peters and Khan, 2015; Scanlon *et al*., 2015; Walker *et al*., 2015; Breedveld, 2013; Aissani *et al*., 2012; Adu *et al*., 2008; Hamzi, Londiche and Bourmada, 2008; Kikuchi, Hirao, 2008; Sugiyama *el al*., 2008a; Sugiyama *el al*., 2008b; Chen, Shonnard, 2004; Flemström, Carlson and Erixon, 2004). The review by Harder *et al*. (2015) specifically focuses on environmental risk assessment and does not cover occupational safety. Occupational safety is an important branch in the field of RA, and the methods concerning health risks in the workplace vary to a great degree in their approach and scope. Hamzi *et al*. (2008) proposed modifying the LCA methodology by including the potential chemical emissions from fire accidents, hence it covers environmental impacts rather than the occupational safety (Hamzi *et al*., 2008). The method by Chen and Shonnard (2004) does not cover accident risks, hence it has been excluded from this study. Khakzad *et al*. (2017) and Strogen *et al*. (2016) suggested merging RA and LCA by monetizing the results of both methodologies. Although the methods developed by Khakzad *et al*. (2017) and Strogen *et al*. (2016) include occupational safety, it was not considered in this thesis due to our understanding that monetary values do not necessarily correspond to the severity of impacts to the AoP, i.e., ‘ignorance of the market’ (e.g., can we monetize the biodiversity loss or human life?). The works by Badr *et al*. (2017) and Sugiyama *et al*. (2008) use hazard (EHS hazards) instead of risk, hence they were not considered in this thesis.

Although the work by Eckelman (2016) does not consider the full risk, the use of Effect Factors (including information about the probability of disease cases per kg intake of a chemical) partly capture the risk from the release of chemicals, hence the method by Eckelman (2016) (the *Life Cycle Inherent Toxicity* (LCIT) method) was considered in this thesis.

1.7.1.Methodology for reviewing the selected life cycle occupational safety methods

As a result of the literature research, three methods for evaluating occupational risks along the life cycle of a product or a service were identified as optimal and selected to be reviewed and compared in our case study: the *Life Cycle Inherent Toxicity* (LCIT) method (Eckelman, 2016), the *Work Environment Characterization Factors* (WE-CFs) method (Scanlon *et al*., 2015), and the *Life Cycle Risk Assessment* (LCRA) method (Aissani *et al*., 2012). The main features of these three methodologies can be seen in Table 1.4. The method by Eckelman (2016) conceptually covers the immediate (acute) and delayed impacts of exposure to organic chemicals caused by accidents or fugitive emissions under normal operating conditions. Due to the lack of connection of non-accidental occupational pressures (e.g., fugitive emissions) to worker health impacts within the EU databases that could be used, the adoption of Scanlon *et al*. (2015) was likely not to include non-accidental health impacts. Yet this is a shortcoming of the EU databases rather than the methodology itself. Aissani *et al*.

(2012) is only concerned about immediate fatal accidents. All the methods are comparative, which means that they do not use threshold values to evaluate the acceptability of the risks, but rather they can be used to compare alternative scenarios. In Chapter 3, the original methodologies were evaluated further by using the case study of pyro-oil production from the *Miscanthus* plant.

Table 1.4. Main features of the selected methodologies

Method	**Eckelman, 2016**	**Scanlon *et al.*, 2015**	**Aissani *et al.*, 2012**
Comparative/Threshold	Comparative	Comparative	Comparative
AoP	Workers	Workers	Workers/Humans
Scope	On-site	On-site	On-site/Off-site
Quantitative/Qualitative	Quantitative	Quantitative	Qualitative
Fatal accident (immediate)	Yes	Yes	Yes
Non-fatal accident (immediate)	Yes	Yes	No
Fatal accident (delayed)	Yes	Yes	No
Non-fatal accident (delayed)	Yes	Yes	No
Fatal disease (no accident)	Yes	No	No
Non-fatal disease (no accident)	Yes	No	No
Agent[1]	Organic chemicals	Many	Many
Data type	Theoretical	Experimental	Theoretical

[1] 'Agent': Cause of the impacts

1.8. Synergistic effects of carcinogenic substances and a logical gap in chemical alternatives assessment frameworks

Article 58(3) of the EU REACH regulation states that the priority for incorporation into the 'authorization list' should be given to SVHC substances that exhibit PBT or vPvB properties or that are being used in high volumes or have wide dispersive use. The direct use of this approach in substitution should be questioned, especially for carcinogenic substances, due to the fact that the regulation focuses on the 'recent' state of the usage, and defines priority substances to be substituted on this basis. There is a logical gap in the application of this approach to chemical alternatives assessment frameworks that might lead to regrettable substitution when the whole life cycle is being considered. As will be discussed shortly with the help of scientific studies on carcinogenicity, the high usage volumes of a specific carcinogen might not be sufficient to justify its substitution, nor can it justify the elimination of the baseline situation without exposing it to equivalent assessments that the alternatives are undergoing.

Although the process of cancer formation is a highly complex issue, literature commonly acknowledges two types of carcinogens. The first type is 'initiators'; these are carcinogens that cause changes to the part of the DNA responsible for cell division, as a mode of action, and mostly are considered mutagenic (Malarkey, Hoenerhoff and Maronpot, 2013; Preston, Williams, 2005). This type of carcinogens covers 88% of all known carcinogens (Hernandez *et al.*, 2009). 'Initiator' carcinogens have virtually no threshold exposure for their effects, and they are relatively less tissue specific

(Malarkey *et al*., 2013). The second type is ‘promoter’ carcinogens which might create favorable circumstances (e.g., allergens, etc.) for cancer initiation.

‘Additive’ interaction means that the effect of two chemicals can be represented by the sum of the effects of each individual chemical separately. ‘Synergistic’ means that, for the same dose, the total effect of two chemicals together is greater than each of their individual effect alone. In other words, these two chemicals enhance each other’s effects. ‘Antagonistic’ is the opposite of ‘synergistic’, meaning that two chemicals can reduce each other’s effectiveness. In most cases, the effect of exposure to two carcinogens is additive, or even synergistic, and only in relatively few cases a slight antagonistic effect is observed (Kawaguchi *et al*., 2006). Another study by the *Norwegian Scientific Committee for Food Safety* points out that additive and synergistic effects might also be dominant in the cases of reprotoxic substances, endocrine disruptors and neurotoxins (VKM, 2008). Hence, additive and synergistic effects should not be ignored. Due to this fact, it is important not only to focus on reducing the chemicals that are being used in high volumes, but it is also crucial to ensure the reduction of the total amount of carcinogenic substances. Recently this important aspect has been lacking alternatives assessments, potentially deeming the policy ineffective.

Also, during the period of 1990–1993, in the EU-15 area, around 32 million workers were exposed to carcinogenic substances, which constituted about 25% of the work force (Eurogip 2010). Despite major improvements, occupational cancer is still an issue today (EU-OSHA 2014). It is clear that any alternatives assessment should not exclude workers in this aspect.

1.9. Wisdom of the crowds effect

There are two kinds of errors that can be made by inexpert assessors: systematic and random. Any method that concerns applicability to SMEs should be evaluated regarding the effect of these errors. The ‘wisdom of the crowds’ effect can be used in error reduction in case of random errors; hence systematic errors cannot be addressed.

The ‘wisdom of the crowds’ effect is a statistical phenomenon that arises from the summation of random choices over a group of probability distributions. This effect is known to reduce overall errors; hence its use has been investigated in many different areas, including genetics (Marbach *et al*., 2012), machine learning (Dietterich, 2000), open source databases (Kittur, Kraut, 2008), finance (Chen *et al*., 2014), and social learning (Golub, Jackson, 2010), to name a few. To the best of the author’s knowledge, this phenomenon has not been investigated in environmental impact assessment or similar areas concerning human and environmental health.

The conclusion section of a paper by Douglas M. Hawkins should be considered in this context: “[…] It is to the effect that Babylonian astronomy, by using a vast accumulation of individually imprecise measurements, was able to make predictions whose quality was not matched by post-Galilean telescopy until about a century ago” (Hawkins, 1991).

1.10. Expert systems approach for environmental impact assessment

Expert systems are defined as computer programs that can emulate the decision-making ability of experts by predetermined programming and databases based on expert knowledge (Jackson, 1998).

A few studies on environmental impact assessment have focused on the ‘expert systems’ approach in parallel with the advancements in computer science (the studies include Ahlmann *et al*., 1992; Hakansson, 2004; Goundar, 2013; Jazzar *et al*., 1998; Lein, 1989; Rachida and Samia, 2013; Say *et al*., 2007), and, to the best of the author’s knowledge, none of them was based on inter-company information sharing for the purpose of performing an LCA.

1.11. Conclusion of the literature review

EU regulations concerning hazardous chemicals set up a well-defined basis for prioritizing the most problematic substances in terms of toxicity and physical hazards or for highlighting some chemicals in terms of risk to the environment, consumers and workers (Section 1.1).

Despite being included in chemical alternatives assessment frameworks, the LCA methodology is not being widely implemented in practice due to resource concerns (Section 1.6). Most frameworks also adopt a preliminary filtering of alternatives based on hazard assessment so that to reduce the number of inputs to their LCA study thus potentially eliminating the better alternatives.

Chemical alternatives assessment frameworks, despite covering a wide scope, still lack quantitative methods addressing life cycle concerns for occupational safety, fugitive and accidental emissions. Furthermore, frameworks do not evaluate baseline situation under the same light with alternative situations (Section 1.6). As mentioned above, this may cause ‘hidden regrettable substitution’, where the collective amount of CMRs might increase although the use/emission of the target SVHC decreases. Our literature review showed that the cumulative effects or amounts of CMR substances should be the basis for evaluation, and, in most cases, synergistic effects mean that impact assessment of carcinogens underestimates the impacts, and this is likely the case for mutagens and reprotoxic chemicals (Section 1.8). However, currently, there is no methodology to account for these synergistic effects, and the best practice is to aggregate their individual impacts over the whole life cycle. This aggregation is currently lacking in the frameworks, except for the carcinogenic effects of intended emissions on the general public (Section 1.6).

Frameworks also need a clearer definition of the scope of impact assessments concerning the life cycle of products/services (Section 1.6.2). Accidental and fugitive emissions should also be considered in environmental impact and occupational safety assessments (Section 1.3).

The reviewed life cycle occupational safety methodologies address physical or chemical risks along the life cycle. Some of these methodologies can be used in combination to address the gaps in the scope of the current chemical alternatives assessment frameworks. The LCIT method is especially suitable for modification as it is based on the intermediate flows of chemicals within the supply chain. These flows can potentially be used to derive generic accidental and fugitive emission amounts (Section 1.7).

The error reduction approaches, such as the 'wisdom of the crowds' effect, that might be beneficial for inexpert assessors as well as expert assessors, are also lacking in the frameworks (Section 1.9 and Section 1.6).

Expert systems regarding inter-company information sharing for the application of environmental impact assessments are also deemed insufficient (Section 1.10 and Section 1.6).

2. Methodology

2.1. Methodological framework

Our methodological framework (Fig. 2.1.) represents the main stages of the doctoral thesis. According to the aim and objectives of the thesis that are determined by the problems detected in the course of the literature review, an environmental impact assessment model has been developed and examined on real case studies. Sensitivity analysis has been performed for uncertainties in assessor inputs due to errors. An error reduction method potentially to be used with the developed model has been proposed.

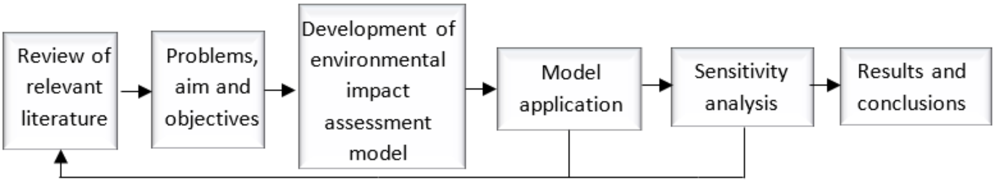

Fig. 2.1. Methodological framework of the doctoral thesis

2.2. Rationale for selecting the assessment methods to be used in the proposed environmental impact assessment model

The methods to be incorporated into the proposed environmental impact assessment model directly or in their modified form were selected according to the following criteria:

1. To be complementary to each other in scope of the impacts covered (i.e., AoP, hazard origin, hazard types and impact pathways covered) to prevent shifting of burden;
2. To be complementary with each other in the spatial scope (i.e., local, regional, and global);
3. To be suitable for streamlining for usage by SMEs;
4. To address the problems identified in the literature review.

2.2.1. Impacts of life cycle emissions and resource extraction

ISO 14044 Standard was adopted as a generic life cycle assessment framework. A generic LCA consists of four phases as seen in Fig. 2.2 (ISO, 2006):

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 LCI phase, the emissions and resources are quantified for the chosen products in the scope of the chosen system boundaries.
3) In the 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 by using previously elaborated scientific models.
4) In the Interpretation phase, for each of the above phases, the outcome is interpreted in accordance with the aim defined in the goal and scope of the study.

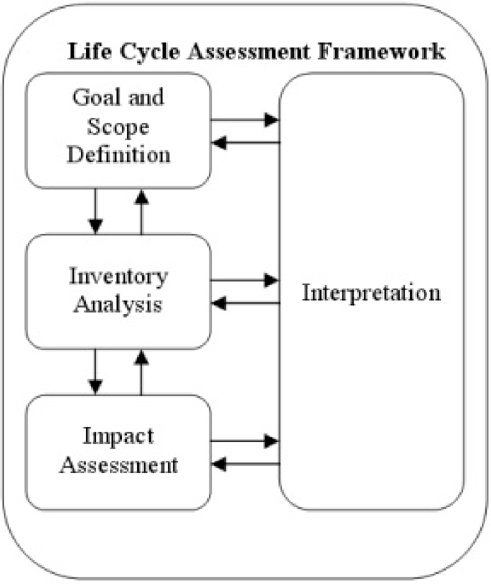

Fig. 2.2. LCA Framework according to ISO Standard (ISO, 2006)

2.2.2. Occupational accidents

Workers represent a sizable share of the mankind; hence they should also be considered as a part of the environment; therefore, the burden cannot be shifted towards workers. Even though, throughout the thesis, environment, humans and workers are mentioned as separate, the author recognizes that these divisions are artificial, and humans as mammals constitute part of the environment.

Under some circumstances, accidents at work have been proved to be as important as the impacts of emission of chemicals (Scanlon *et al*., 2015), hence the WE-CFs method was adopted to address this issue.

Further examination of life cycle occupational safety methodologies and rationale for their selection was performed in Chapter 3 in more detail.

2.2.3. Intermediate chemicals

Toxicity impacts of life cycle intermediate chemicals on workers should be addressed; hence the use of the LCIT method was found to be necessary (see Section 1.11, Section 1.8 and Section 3.4). Further examination of life cycle occupational safety methodologies and the rationale for their selection was performed in Chapter 3 in more detail.

2.2.4. Accidental and fugitive emissions

Impacts of the life cycle fugitive and accidental emissions on the environment should be evaluated (see Section 1.3). The simplified LCA deals with the intended emissions, hence the LCIT method had to be modified to address this gap in environmental impacts (see Section 1.11).

2.2.5. Usage amounts

The simplified LCA covers neither life cycle intermediate chemicals nor their effects on workers. Also, the WE-CFs method dealing with physical accidents does not cover chemical hazards, either. The LCIT method only addresses known carcinogenic substances and traditional toxicity impacts. Hence, it is necessary to include the impacts on workers exerted by the chemicals that are not covered by other methods employed in this thesis. Preferably, additional relevant chemical hazards should include reprotoxic, highly flammable/reactive/explosive hazards (see Section 1.6.2). Also, suspected carcinogenicity and mutagenicity should be accounted for (see Section 1.8). For the above mentioned hazard categories, currently, there are no impact assessment methods available, hence only usage amounts can be used as a measure of hazard.

2.2.6. Emission amounts

The emission amounts of those substances that are not addressed by the Simplified LCA were necessary. The simplified LCA currently does not account for suspected carcinogens/mutagens, reprotoxics, or bioaccumulation hazards (see Section 1.11).

2.2.7. Local and regional environmental impacts

RA was necessary to address the risks of hazardous substances on workers of the company and the consumers of the product, as well as the risks imposed on the local/regional ecosystems (see Section 1.7).

2.3. Selection of representative processes

The selection of representative processes is necessary due to the limitations of manual assessment that requires evaluation (e.g., classification into economic activities, obtaining USEtox effect factors, etc.) of thousands of unit processes (6,037 unit processes for each case) in LCI. Currently, there is no software available for automatically performing the proposed environmental impact assessments. Due to this limitation, representative processes were chosen to be representative of the complete LCI. As the number of representative processes was unknown, the LCI database was examined to determine the optimum number of processes to be used as a representative of the complete LCI. For climate change, the percentage contribution of the topmost contributing 10, 20 and 40 major processes was selected and evaluated for their representative accuracy. The processes contributing to the climate change directly or indirectly were also taken into account. In other words, a process that does not emit greenhouse gas emissions directly, but through energy usage from the electricity grid, was taken into account within the source of these emissions. Furthermore, the representative processes for climate change impacts were assumed to be the same for other impact categories as well. This assumption is based on the work of Huijbregts *et al*. (Huijbregts *et al*., 2010; Huijbregts *et al*., 2006) concluding that, currently, the energy consumption is proportional to the climate change impacts.

2.4. 'Inexpert outcome' systematic error evaluation

To evaluate the suitability of the proposed environmental impact assessment model for inexpert assessors with regards to the involvement of systematic errors, systematic error evaluation was needed (see Section 1.9). The simplified LCA as a part of the impact assessment module as defined in Section 4.1.3.1 will be used to examine the effects of systematic errors (in combination with or without random errors) of an inexpert assessor as a form of sensitivity analysis (see Fig. 2.3).

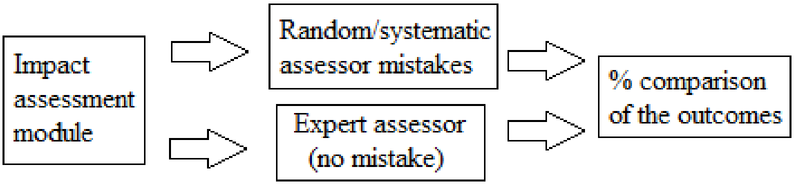

Fig. 2.3. 'Inexpert outcome' systematic error examination module

2.5. 'Inexpert outcome' random error evaluation

The 'wisdom of the crowds' effect as described in Section 4.2 was proposed as a framework for the evaluation of random errors made by inexpert assessors. This was necessary for the evaluation of the effect of potential random errors on assessment outcomes and for the examination of potential improvements in error reduction strategies by using statistical methods (see Section 1.9).

2.6. Use of multi-criteria decision analysis

The use of multi-criteria decision analysis (MCDA) was not preferred to be employed for decision making due to the unscientific aspects of the MCDA method regarding its application to the proposed environmental impact assessment model. Although the MCDA method is being widely used (Huang, Keisler and Linkov, 2011) due to the lack of purely scientific solutions, the author stresses that MCDA is not the appropriate method to be used for environmental impact assessment purposes, especially when economic indicators are being used. The practices that apply MCDA for decision making involving economic and environmental variables lack solid scientific ground. This is especially clear when economic assessments base themselves on economic growth by using payback period indicators. If the goal of environmental and economic assessments is to increase the well-being of humans and the environment, then the payback period indicator is not a good measure as it bases itself on the growth paradigm rather than on sustaining the economy. According to this outdated indicator, one can disregard any alternative that pays itself back in the long-term, which leads to ‘no growth’ in economy. This does not mean that the business is unsustainable, nor that it is not creating a better world. It just means that it is not growing as a natural system. If the payback period indicator were applied to ecosystems, we would replace all the ecosystems with businesses that bring more economic growth, which, in fact, is what we are doing. There are many clear scientific arguments against the growth economy; however, that is where the politics of power structures come into play to distort science (McNeill, 1999). Also, there is no correlation between the price of a product and its importance for human well-being, as – today – consumption is heavily culturally driven (particularly in the ‘developed countries’) based on ‘wants’ rather than ‘needs’.

Another point is that, when the price of a product goes up due to the consideration of an environmentally better performing alternative, the producers of the products already have a rough idea on how much price increase is too much to render them out of business. This is the same for the technical performance of a product to perform a given function; producers already have a rough idea of the minimum performance requirements for their products. So, instead of performing MCDA among unrelated criteria whose effects on AoP are not well-established, we should define an acceptable range for the technical performance and economic costs for a given product and take the rest of the decisions based on environmental impact assessment.

Apart from the inconvenience of using payback period or other monetary concerns in MCDA, there is a more fundamental problem with the MCDA method applied to decision making for environmental concerns. The fundamental problem is that, except for the case of which the minimum values could be found for all impact categories for a given scenario, the normalized and weighed results of different units are scientifically meaningless unless they are derived with scientific reasoning. The issue is not even related with the usage of arbitrary cultural ‘weights’ for aggregation, it is the fundamental shortcoming that each individual assessment (Simplified LCA, modified LCIT, etc.) measures different aspects towards environmental impacts, and thus there is no established scientific connection between them and the well-being and sustainability of the AoP. However, normalization can be performed semi-scientifically, by using logic and assumptions.

It can be shown that, for a situation where impacts from all indicators are minimal for all the scenarios, comparisons to other scenarios are the only situation where MCDA would certainly be meaningful. To show this from a statistical perspective, let us assume a matrix of alternative scenarios (a_n) and indicator categories (i_m), as shown in Eq. 2.1.

$$\begin{array}{cccc} - & a_1 & a_2 & a_3 \\ i_1 & 11 & 12 & 13 \\ i_2 & 21 & 22 & 23 \\ i_3 & 31 & 32 & 33 \end{array} \qquad \text{(Eq. 2.1)}$$

The only circumstance where the preferred scenario would be scientifically meaningful is the scenario that has the minimum indicator values for all the indicators compared to all the other scenarios. This can also be named as a normalization/weight independent pareto solution. The question is under which circumstances it is highly likely that an alternative scenario would have the minimum values for all the indicator categories. If we assume that indicators are independent from each other, then each indicator for each scenario would have $1/n$ probability of being minimum for a given indicator category. For a given scenario, the probability of all the indicators being minimum is given by $(1/n)^m$. Due to the fact that there is no preference for a specific scenario, the probability of having all the indicators minimum for a given scenario becomes $m(1/n)^m$. If we agree on 95% chance of finding all indicators minimum for any one scenario as an acceptable chance of MCDA being valid, then this can be expressed as in Eq. 2.2.

$$n^{(1-m)} = n(\frac{1}{n})^m \geq 0.95 \qquad \text{(Eq. 2.2)}$$

According to Eq. 2.2, as m and n are integers that are always equal to or bigger than 1, it is obvious that no multiple scenario condition satisfies Eq. 2.2. Hence, it can be concluded that the use of MCDA for indicators without science-based normalization and weightings is meaningless. Therefore, normalization factors should be derived based on scientific reasoning.

Due to lack of a better solution, normalization of the results usage/emission amounts method could be done (except for explosion/fire hazards) by using average characterization factors of chemicals with non-zero characterization factors in the LCI database of the ReCiPe 2008 method (ReCiPe, 2009). Non-zero values could be chosen because it is known or suspected that, for chemicals that are in the usage/emission amounts method results, hazards *do* exist. Hence, a characterization factor of 1.2E-6 DALY/kg emitted could be assumed as a normalization value for emission amounts method outcomes, derived by median characterization factors of chemicals due to emissions regarding each of the 7 sub-compartments as a subdivision of 3 compartments (i.e., air, soil and water) (See Fig. 2.4). For the usage amounts method, if we assume that reprotoxics, endocrine disruptors and suspected carcinogens all have similar impacts as carcinogens, then, the normalization factor of 1.30E-5 as derived below for the LCIT method inhalation cancer impacts can be used after multiplying with the average inhalation cancer effect factors of common chemicals. Chemicals in the four selected company cases were used for this purpose (see Section 5.1 for cancer effect factors of various chemicals as a result of the LCIT method). The average of the inhalation cancer effect factors (with only non-zero values included) was found to be 1.95E-2. Hence, the factor of 2.54E-7 DALY/kg usage was obtained by multiplying the average of the inhalation cancer effect factors with 1.30E-5. However, due to the very large uncertainty, these normalizations were not suggested by the author.

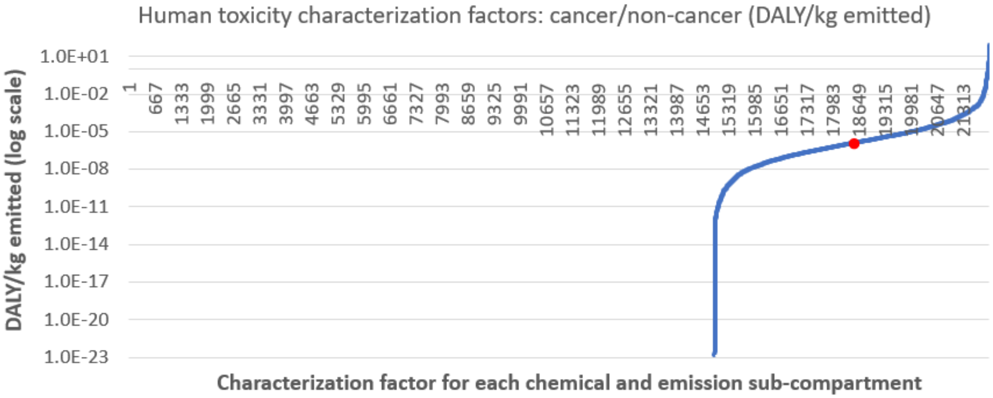

Fig. 2.4. Human toxicity characterization factors (total of 21,973; zero values are not shown) of approximately 3,000 chemicals, for emissions to each of the 7 sub-compartments, in the LCI database of the ReCiPe 2008 method (ReCiPe, 2009); the red dot shows the median of non-zero values

For the LCIT method, normalization was done by using cancer/non-cancer disease case to DALY conversion values proposed by Huijbregts *et al*. (Huijbregts *et al*., 2005). These values are 11.5 DALY/disease case for cancer effects and 2.7 DALY/disease case for non-cancer effects. As LCIT results are for kg of intake of substances, an emission factor of 1.90E-3 should be applied (see Step 23 in Section 4.1.6). Also, the worker exposure factor was approximated by assuming a workplace indoor volume of 350 m^3 (Fantke *et al*., 2017). Indoor emissions for each day were assumed to be released into a ventilated (4200 m^3/hour/person) industrial workplace with 1 worker working 4.76 hours per day and having an inhalation rate of 2.5 m^3 per hour (Fantke *et al*., 2017). Use of Eq. 2.3 (Fantke *et al*., 2017) yielded the total inhalation value of 5.95E-4 kg per worker per each kg of volatile/gaseous substance(s) emitted. As the air volume in the workplace was assumed to be proportional to the workers, emissions – whether being company specific or distributed along the life cycle – do not affect the obtained results. Dermal exposures from fugitive emissions are also being neglected in our research.

$$Exposure = \frac{M \times IR \times N}{V \times m \times k} \qquad \text{(Eq. 2.3)}$$

Here, M is the mass emitted indoors per hour, IR stands for the inhalation rate of each worker, N denotes the number of workers, V is the volume of the indoor air, m is the mixing factor (shall be assumed to equal 1), and k is the indoor air ventilation rate ($k=12\ h^{-1}$ for industry in OECD countries (Fantke *et al*., 2017)).

Hence, the LCIT method cancer results should be multiplied by 1.30E-5 (=11.5*1.90E-3*5.95E-4), and the LCIT non-cancer results should be multiplied by 3.00E-6 (=2.7*1.90E-3*5.95E-4) in order to convert their units into DALY.

2.7. Harmonized internet system for life cycle assessment: expert systems approach

It has been recognized by the author that presenting an environmental impact assessment model without addressing its practical application concerns is incomplete.

Hence, the expert systems approach should be adopted to further overcome the scarcity of resources and expertise for performing LCA. Although an expert system has been proposed to improve the practical application of LCA, expert systems can be developed for the application of the proposed environmental impact assessment model.

To achieve this, companies would be obligated to fill in an online form regarding the process data that is necessary to perform the proposed environmental impact assessment model. By taking notice that the major companies should already have their input-output and product information under a permit, such as the Integrated Pollution Prevention and Control (IPPC) permit (EU, 2010c), a system has been proposed (the Harmonized Internet System for the Application of LCA, shortly named as HIS-LCA) to be applied to the whole industry.

Also, the use of the 'combined total functional demand' regarding the total output of the technosphere was necessary to track changes caused by the substitution thus enabling evaluation of the downstream changes caused by the substitution.

3. Evaluation of Occupational Life Cycle Methodologies

Unlike other well-known methods (such as LCA and RA) employed in the environmental impact assessment, occupational life cycle methods had to be evaluated in a preliminary case study (pyro-oil production from the *Miscanthus* plant) in terms of their suitability for the goals of this thesis.

3.1. Description of life cycle occupational safety methodologies to be evaluated for incorporation into the developed environmental impact assessment model

In this section, the selected life cycle occupational safety methodologies are briefly explained. For a detailed description of these methods and definitions in use, the original studies may be referred. The incorporation of these selected methods into the developed environmental impact assessment model was conducted after the examination of the suitability of these methods on a preliminary case study (pyro-oil production from the *Miscanthus* plant) and the appropriate modifications.

Life cycle inherent toxicity (LCIT) method

The method is influenced by the green chemistry principle which suggests reducing the inherent hazard of chemicals used in the processes in order to be able to reduce the occupational risks, either from acute exposure, or from fugitive emissions associated with the use of these chemicals. This method uses intermediate chemical (organic chemicals) flows as the inventory while assuming that the risks from exposure to these chemicals are proportional to the amount of the chemical(s) used in each unit process and to the toxic effects of those chemicals; hence, we take a different approach in comparison to that of the conventional LCAs which focus on emissions to the environment or inputs from the environment in order to assess the impacts on humans (but not on workers) via different exposure routes. The method accounts only for the organic chemicals as the uncertainties related to the impacts of other chemicals, such as metals (Hauschild *et al.*, 2013) and nanoparticles, currently still need improvement.

The use of USEtox® (USEtox, 2017; Rosenbaum *et al.*, 2011) for the calculation of characterization factors for organic chemicals was adopted by this method. USEtox® is a steady state ‘multi-compartment model’-based quantitative impact assessment method for calculating the impacts of released chemicals on humans and environment (more specifically, on living species). For humans, USEtox® can calculate the cancer/non-cancer disease cases per kg of chemical released to a specific compartment by using inhalation/ingestion effect factors (Jolliet, Fantke, 2015; Rosenbaum *et al*., 2011). Severity factors are the weightings that reflect the severity and seriousness of the disease. UseTox® only calculates the disease cases per kg of chemical(s) emitted (in units of Comparative Toxic Unit for human (CTUh)). In the case of Effect Factors, UseTox® also calculates the disease cases per kg of chemical intake (CTUh (intake)). However, UseTox® results do not include the severity factors (Jolliet, Fantke, 2015). Thus, aggregation of the results for cancer and non-cancer cases should not be performed.

Lastly, the corresponding effect factors were multiplied with the intermediate flows in order to calculate the inherent toxicity impact scores for each impact category. Aggregation over the same disease type (cancer or non-cancer) and exposure route (inhalation or ingestion) over the whole life cycle should be performed.

WE-CFs method

In contrast to the traditional LCA impact assessment methodologies, this method uses a different approach towards the calculation of endpoint impacts on humans. Instead of rigorous systematic calculation of the impacts derived from hazardous chemicals, the method simply bases itself on the endpoint observational data (disability adjusted life years (DALYs) for work environment) for each industry branch, and subsequently scales the impact score to the output of each unit process classified under that branch.

Classification of the identified processes into industry activity branches is needed (for the EU economic activities, currently NACE Rev. 2 classification (Eurostat, 2008); for USA, NAICS (Scanlon *et al*., 2015) are used).

Literature and databases were searched for information related to production amounts and Years of Life Lost (YLL) and Years Lost due to Disability (YLD) calculation for the identified industry branches (for the EU, NACE Rev. 2 activities; for USA, NAICS), and the gross WE_DALYs for each branch as described by Scanlon *et al*. (Scanlon *et al*., 2013) was calculated.

LCRA method

The method follows the traditional LCA framework as a template for its structure. It qualitatively (in the form of levels) assigns occurrence probabilities to hazardous situations, categorizes hazardous situations into hazard categories (e.g., explosion, physical trauma, inhalation, etc.), and assigns an extent of damage that might result in fatal accidents stemming from these situations. It uses qualitative functional units to compare the occupational risks of different products/services that serve the same function.

The occurrence probabilities are assigned with a method similar to Event Tree Analysis (with assigning predefined relative generic probabilities of failure for different combinations of independent sub-processes and only taking the first tier for the sake of simplicity), while the extent of the damage that can cause fatal accidents is represented by the physical space affected, more specifically, by the nature (on-site/off-site) of the area affected by the accidents.

Probability levels (Levels 1,2,3) and the extent of the damage (Levels 1,2) are assigned to each classified accident by investigating these sub-processes further for the number of 'necessary elements' for the accident(s) to happen and the extent of damage onsite or off-site. These levels are defined by Aissani *et al*. (2012) (also see Fig. 3.1).

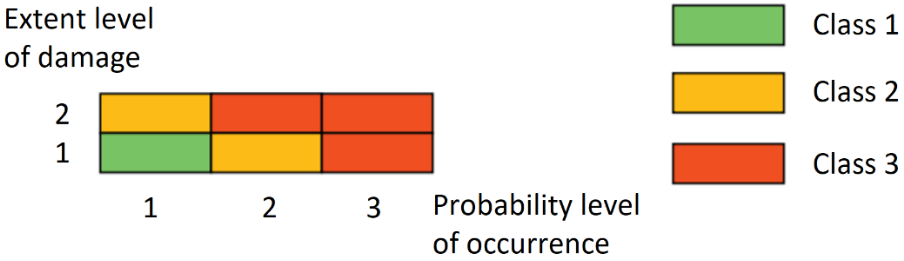

Fig. 3.1. Classes of risk (Aissani *et al*., 2012)

The overall score is given by Eq. 3.1:

$$\frac{((m_1 x1)+(m_2 x2)+(m_3 x3))}{(m_1+m_2+m_3)}; \qquad \text{(Eq. 3.1)}$$

here, m_j – the number of accidents of risk class j as defined in the previous step.

3.2. Description of the system used for the case study for life cycle occupational safety methods

A simplified life cycle of the electricity production from pyro-oil derived from the *Miscanthus* plant was adopted to be used in the preliminary case study to examine the suitability of life cycle occupational safety methods. The main processes are outlined in Fig. 3.2. The main processes include the cultivation of the *Miscanthus* plant, its transport to pyrolysis, pyrolysis of the *Miscanthus* plant, transport of the pyrolysis oil to an electricity generation plant, and burning of pyrolysis oil to obtain 1 MJ of electricity.

For electricity and heat production inputs to the drying, grinding and pyrolysis processes, the databases in SimaPro (SimaPro version 8.4.0.0) were used (SimaPro, 2017). For the baseline scenario, electricity production processes were represented partially by the “Electricity, high voltage {IT} production mix, Alloc Def, U,”. Inputs to heating processes were represented partially by the “Heavy fuel oil {Europe without Switzerland} market for Alloc Def, U” process. A 5% cutoff value for CO_2 emissions and the exclusion of the infrastructure processes have been adopted. The full process chains were not used; instead, the major processes with a significant amount of intermediate flows (more than 10E-6 units) were considered. The efficiencies and heating values were sourced from the ELCD database (JRC, 2017), except for the heating value for petroleum (43 MJ/kg) (WNA, 2016).

The remaining segments of the processes diagram were adopted from the work of Paolucci *et al*. (Paolucci, Bezzo and Tugnoli, 2016).

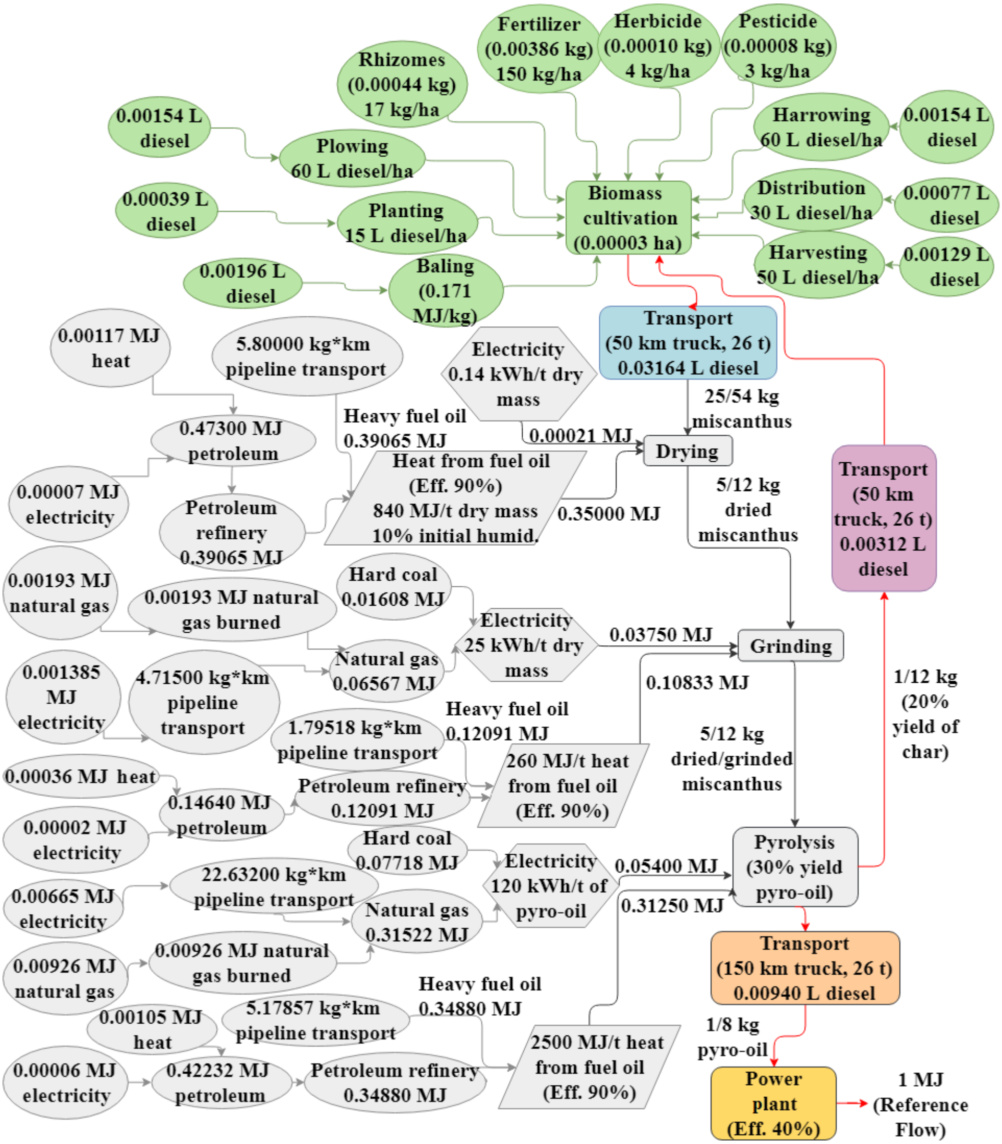

Fig. 3.2. Major life cycle processes of electricity production from pyro-oil (color codes are defined for Chapter 3 independently from any other sections of this thesis)

3.3. Application of life cycle occupational safety methods to Miscanthus case study and the results

Life cycle inherent toxicity method

On the grounds of data covered in Chapter 3 and the original study:

The scope was defined as in Fig. 3.2 (see Annex I). The functional unit was defined as “the production of 1 MJ of electricity.” Hence, the reference flow was defined as “1 MJ of electricity.”

The organic intermediate flows that are considered to be inherently unsafe for the considered hazards (i.e., inhalation/ingestion cancer/non-cancer toxicity) are herbicide, pesticide and pyro-oil. Diesel fuel and fuel oil which can be represented (HHS, 1995; Date, 2011) by Alkenes C15–C18 (Cas No. 93762-80-2) had no effect factors in the USEtox® database as diesel fuel is not considered to be toxic and accidental poisoning is very rare (HPA, 2006). For petroleum, it is more difficult to assess the toxicity since its composition is much more complex (HHS, 1995).

Although the composition of pyro-oil depends on many factors (such as the process temperature, the type of plant, etc.), assigning representative composition for the toxic components of pyro-oil (Mullen, Boateng, 2008) was still possible.

Representative chemicals for the identified organic intermediate flows are listed in Table 3.1 (for details, see Annex I).

The effect factors for the identified chemicals were imported from USEtox® (for release into indoor air) as outlined in Table 3.2 (for details, see Annex I).

Aggregation over different exposure routes (i.e., inhalation, ingestion) for the same disease type (cancer or non-cancer) was applied separately for each life cycle stage; agriculture (diesel, fertilizer, herbicide and pesticide productions as sub-processes), transport to pyrolysis, overall pyrolysis (including drying and grinding), pyro-oil transportation, bio-char transportation, and electricity production. The amounts of intermediate flows were calculated by using Fig. 3.2 and Table 3.1 (see Annex I). The results are outlined in Table 3.3 (see Annex I).

WE-CFs method

The scope was defined as outlined in Fig. 3.2. The functional unit was defined as “the production of 1 MJ of electricity,” hence the reference flow was defined as “1 MJ of electricity.” The process network and the related quantitative intermediate flow information is presented in Fig. 3.2.

Classification of the processes within the defined scope (see Fig. 3.2) into industry (economic) activity branches is outlined in Table 3.4 (see Annex I).

In the process of searching for suitable online databases, the encountered relevant databases were examined for the availability of information related to YLL and YLD caused by occupational accidents in EU-28. It was thus possible to compile data for the calculation of YLLs as described by Scanlon *et al*. (Scanlon *et al*., 2013) (for details, see Annex I). In the Eurostat database (Eurostat HSW, 2017), the *accident at work* is defined as “a discrete occurrence in the course of work which leads to physical or mental harm.” In the database, only fatal and non-fatal accidents involving more than 3 calendar days of absence from work are included.

Production amounts for each economic sector (Table 3.5) were extracted from Eurostat databases (for details, see Annex I).

WE_DALY values (Table 3.6 in Annex I) were multiplied with the corresponding output amounts (as shown in Fig. 3.2) so that to obtain the WE_DALY impact scores (see Table 3.7 in Annex I).

The total WE_DALY score for 1 MJ electricity production from pyro-oil is 1.27E-08 years.

LCRA method

The scope was determined as the processes depicted in Fig. 3.2. The functional unit was qualitatively determined as “the production of electricity.” The process network is presented in Fig. 3.2. Dangerous situations and related accidents were investigated on the grounds of the data outlined in the thesis by Aissani (Aissani, 2008), the Eurostat database (Eurostat HSW, 2017) under the dataset names “Accidents at work by sex, age, severity, NACE Rev. 2 activity and contact mode of injury,” and “Accidents at work by sex, age, severity, NACE Rev. 2 activity and material agent of contact mode injury.” Also, the U.S. National Agriculture Safety Database (Runyan, 1993) was used. The inventory table of dangerous situations and related accidents was formed (see Table 3.8 in Annex I) on the basis of the data from the previous step. The obtained results can be seen in Table 3.9 (see Annex I), Table 3.10 (see Annex I), and Table 3.11.

Table 3.11. Summary of the percentage contribution of risks to each life cycle stage for each method

Life cycle stage		Agriculture	Transportation to pyrolysis	Overall pyrolysis	Pyro-oil transportation	Bio-char transportation	Electricity production
LCIT	**Cancer**	0	0	0	50	0	50
	Non-cancer	4.4	0	0	47.8	0	47.8
WE-CFs		90.7	2.0	4.8	1.6	0.4	0.6
LCRA score		11.7	20.8	15.6	20.8	20.8	10.4

3.4.Discussion and conclusion of the evaluation results of life cycle occupational safety methods on preliminary case of pyro-oil production from Miscanthus plant

Discussion

In the LCIT method, the inclusion of exposure factors for human toxicity derived from USEtox® seems irrelevant for occupational safety as the exposure pathways between the compartmental concentration-general public and compartmental concentration workers are fairly different, hence, the use of fate factors as standalone is the most convenient approach. This method does not include exposure as it does not use exposure scenarios. The results of the method are highly heterogeneous, and the major cancer and non-cancer impacts originate from the same life cycles.

The WE-CFs method generalizes the risks within each economic sector and extrapolates previously observed risks in various economic sectors to the current situation. The results (as seen in Table 3.11) are highly heterogeneous over the life cycle of electricity production from the *Miscanthus* plant. Agriculture is the most prominent contributor to the occupational risks. The method does not take into account the life years lost from fugitive emissions as the method is only concerned about the cases of "discrete occurrence in the course of work which leads to physical or mental harm." Even if the method included a broader definition of an accident, the connection between the occupational conditions and the disease would mostly be subtle, and the relation(s) of diseases to the occupational conditions is/are often not reported.

In the LCRA method, the occurrence probabilities are generically defined and assigned with a method similar to the Event Tree Analysis (with assigning predefined relative generic probabilities of failure for different combinations of independent sub-processes and only taking the first tier for the sake of simplicity), while the extent of the damage that can cause fatal accidents is represented by the physical space affected (the spatial extent), more specifically, by the nature (on-site/off-site) of the area affected by the accidents. Also, the use of a functional unit is qualitative; hence, the cases that perform the same function can be compared. However, the method is based on qualitative data. Therefore, some important aspects (reference and intermediate flow amounts) are missing. Furthermore, the outcome of the method highly depends on whichever sub-processes are being included, irrespective of the fatality contribution of the sub-processes. In other words, the probabilities or frequencies of fatal accidents cannot be used in the method. The most obvious shortcoming of the method is that it averages the individual risks rather than sums them when obtaining a single score. Although, for low probability events, it may be a good approximation for comparison between different risk classes that contain a similar number of sub-processes, this averaging causes the information about the frequency of the risks over a life cycle to be lost. To depict this more clearly, let us assume a system that has 2 processes of Class 1 and one process of Class 2, with 'Classes' being defined as in Fig. 3.1. The overall score for this system would be 4/3 (approximately 1.3), as overseen by Eq. 3.1. Now, if we consider another system that involves 5 processes of Class 1 and one process of Class 2, then, the overall score for this latter system would be 7/6 (approximately 1.17). As it is clear that the latter system has 3 extra processes of Class 1 (which adds to the risk), inherently, it should yield a higher risk score, yet, the results of the LCRA method wrongly tell us that it features a lower risk score. Similarly, in Table 3.10, pyro-oil transportation and bio-char transportation processes have the same LCRA score although pyro-oil transportation includes an extra risk of an accident of fire. These are cases of bargaining between accuracy and simplicity that may cause systemic errors for a given case. The results stemming from this method are quite homogeneous among life cycles due to the averaging effect.

Conclusion

Each method has its own advantages and disadvantages. LCIT is the simplest method among the three methods, and also the easiest to apply. It covers the accidental and non-accidental situations where exposure to organic chemicals might potentially take place. A major downside of the method is the lack of inclusion of exposure risk. The WE-CFs method has a potential to be applied in more detail if the detailed occupational safety databases, the careful follow-up and analysis of diseases in workers and the detailed and accurate reporting are represented. Our work shows that it is possible to apply this methodology for the EU-28 region. The LCRA method was found to be highly ambiguous due to the effects of averaging, lack of the use of quantitative reference flows and the variety of accidents that can be involved. Also, the application of the LCRA method is not straightforward as it is a simplification of an extremely complex issue and thus can require more time if compared to the two other methods; subsequently, it might need the highest expertise levels in comparison to the other methods regarding various details of the processes. Due to these observations, this particular method was not considered to be used in the developed environmental impact assessment model.

All the methods are comparative methods, which suggests that they do not use thresholds. Hence, none of the methods can evaluate whether the risks are acceptable.

Overall, methods yield different results due to the differences in their scope and assumptions.

4. Development of the Environmental Impact Assessment Model for Substitution of Hazardous Substances

4.1. Explanation of the proposed thesis model for impact assessment

The aim of the model is to assess environmental impacts of substitution of hazardous substances in industrial companies.

To achieve this, inclusion of the simplified LCA was necessary as it was the only well-established methodology that accounts for the environmental and human health impacts of pressures along the whole life cycle. As stated by Jacobs *et al.*: "What is clear in the rationale for adopting life-cycle thinking is the need for a more streamlined approach to identifying life-cycle impacts. However, greater methodological clarity about what is encompassed in life-cycle thinking would be of benefit to the alternatives assessment field" (Jacobs *et al.*, 2016). Also, the simplified LCA covers carcinogenic substances, hence it directly addresses a part of the SVHC in a wider life cycle scope. The WE-CFs method was adopted due to its coverage of human health impacts stemming from occupational accidents along the upstream life cycle. Currently, alternatives assessment frameworks ignore the worker health and safety issues outside of the company boundaries. The LCIT method was adopted for its coverage of occupational hazards due to fugitive or accidental emissions along the life cycle – for the same reason as mentioned regarding the WE-CFs method. The modified LCIT method was proposed to target the gap in the scope of the three other methodologies, namely, human health and environmental impacts from potential fugitive emissions and emissions caused by accidents along the upstream life cycle, which is currently not being covered by the existing alternative assessment frameworks. Frameworks usually focus on relative exposure assessments seeking to reduce risk and on such parameters as physicochemical properties, use characteristics, emissions and fate, and industrial hygiene measures. It was recognized that performing risk assessment with ECETOC TRA software would not add much complexity to the already existing exposure assessments which evaluate relative risks. Risk assessment (ECETOC TRA as suggested by ECHA for the EU region) was employed not in order to ensure that the chemical toxicity risks are acceptable, but rather to be used for relative comparison. Yet, the results also indicate unacceptable risks when risk characterization ratio (RCRs) values exceed 1. An additional assessment step was added for use and emission amounts of substances in order to address the gaps (reprotoxicity, endocrine disruption, highly flammable/explosive/reactive, carcinogenic/mutagenic substances) in other proposed assessment types. All the assessments were accumulated in a parallel manner, and their scope can be seen in Table 4.1.

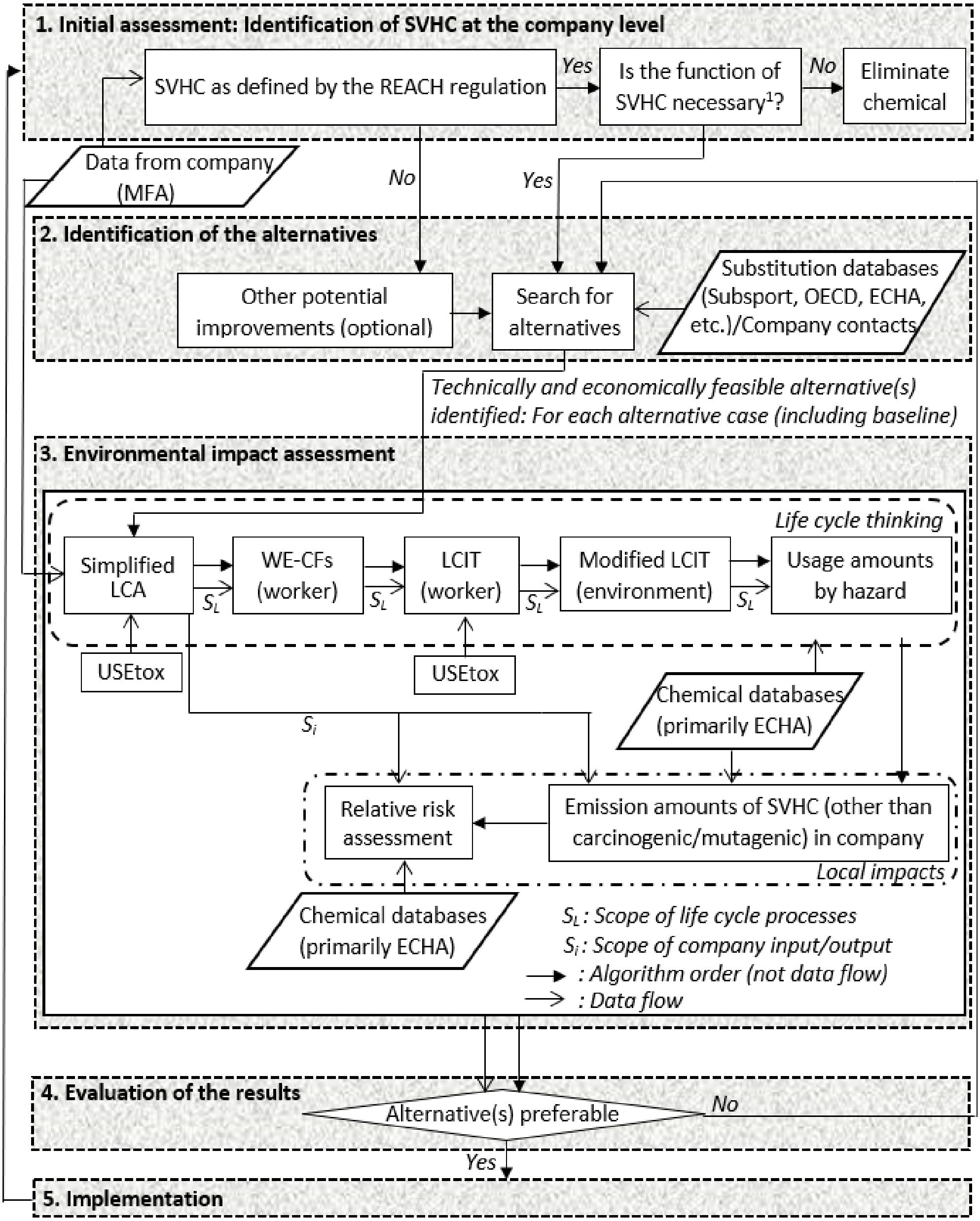

Fig. 4.1. Environmental impact assessment model for substitution of hazardous substances by using the life cycle approach. ¹'Necessary': chemicals which serve a mandatory function in really indispensable products/services; products/services which human well-being would be negatively affected due to lack of an alternative cultural/technical solution when their supply is hindered

The method accounts for the substances in the candidate list of substances of very high concern, and any article or mixture that contains more than 0.1% w/w of the SVHC substances is being considered as necessary to substitute. The model isd intended to be used by mixture and article producers, as well as by chemical manufacturers. In the case of chemical manufacturers, synthesis of a new alternative chemical might delay the alternatives assessment process until the chemical properties of this new chemical have been evaluated.

Table 4.1. Scope of individual assessments as part of the proposed environmental impact assessment model

	Simplified LCA	**LCIT**	**Modified LCIT**	**WE-CFs**	**RA**	**Usage amounts**	**Emission amounts**
Life cycle thinking	✓	✓	✓	✓		✓	
Environment	✓		✓		✓		✓
General public	✓		✓		✓		✓ [1]
Consumers					✓	✓	
Workers		✓		✓	✓	✓ [2]	
Physical hazards				✓		✓ [3]	
Fugitive/accidental emissions			✓				

[1] Reprotoxic/endocrine disruptor/suspected carcinogen/suspected mutagen/PBT/vPvB;

[2] Reprotoxic/endocrine disruptor/suspected carcinogen/suspected mutagen;

[3] Highly flammable/explosive/reactive

4.1.1. Initial assessment: Identification of SVHC at the company level

The goal of the model application should be defined. The goal of the model application can be worded as “to reduce hazardous substances used in the company C and in its supply chain without increasing the environmental impact of the target product P.” Here, the target product is a product that uses the identified SVHC. Company level MFA should be performed (for each production process) and compared to the already existing SVHC lists so that to identify any SVHC. The ECHA database provides comprehensive information on CMR, PBT/vPvB, endocrine disruptor properties of substances that renders them SVHC. The authorization list, the candidate list and the restriction list by ECHA, or any other lists concerning SVHC by widely recognized organizations, such as by the ChemSec Sin list (ChemSec, 2019), can be used to identify SVHC used in the company. Optionally, a flowchart of the process that uses SVHC can be requested from companies by assessors to help understand the situation better.

4.1.2. Identification of alternatives

Identification of alternatives to hazardous substances for a given use in a particular production process can be done in various ways. *Subsport* is a database dedicated for this purpose (Subsport, 2016c). ECHA also has a dedicated online section on their webpage (ECHA, 2019c). In addition, companies can rely on their company contacts, internal researchers or various seminars held for dissemination of substitution practices in companies.

In the case where no SVHC was identified in the company as a result of MFA, the company can optionally choose to perform the model for other potential improvements (e.g., the company might want to reduce the life cycle impacts in general, etc.) concerning hazardous substances other than SVHC as defined in this thesis.

Alternatives, in addition to being economically feasible, should meet performance expectations and standards set by regulations (if any).

4.1.3.Environmental impact assessment

4.1.3.1. Simplified life cycle assessment

The selected method for deriving LCA indicators is ReCiPe 2016 (Huijbregts *et al.*, 2016). This choice was made because the ReCiPe methodology represents the most recent progress in life cycle impact assessment methods, covers a wide range of impact categories, and concerns the European region.

The comprehensiveness of an LCA is defined by the scope of its system boundaries (which processes of the life cycle are included), the considered input-output types, and the selection of impact categories. For the application of LCA in this thesis, a case specific inventory for the examined processes is used, complemented by the industry average data for the rest of the life cycle (EeBGuide Project, 2012).

Detailed description of each impact category and methods is provided in the work of Huijbregts *et al*. (Huijbregts *et al*., 2016). Impacts on the environment, resources and human health are usually evaluated by the following scheme (Fig. 4.2):

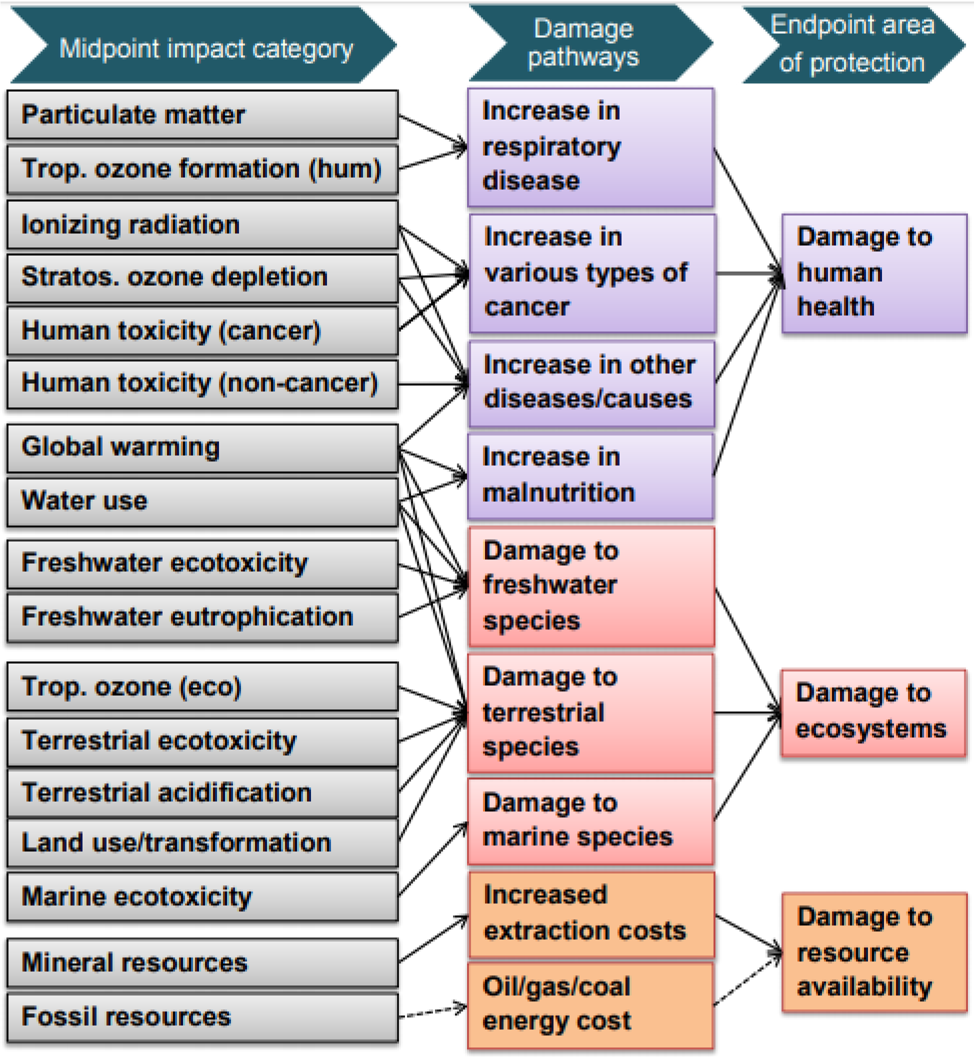

Fig. 4.2. Common LCA methodology connecting LCI to impact indicators (Huijbregts *et al*., 2016)

The ReCiPe 2016 endpoint impact methodology is explained below.

The general structure for the calculation of impacts, both endpoint and midpoint, in the ReCiPe 2016 method is given in Eq. 4.1.

$$Impact = Amount\ emitted\ \times Charactrization\ factor \qquad \text{(Eq. 4.1)}$$

Due to length limitations, it is impractical to give all the equations that were used in the calculation of Simplified LCA endpoint impacts in this thesis. However, readers can refer to the ReCiPe 2016 methodology (Huijbregts *et al*., 2016) for more details.

4.1.3.2. WE-CFs method

WE-CFs method results (in DALY units) are calculated by using Eq. 4.2:

$$Impact\ WECFs = \sum_s m_s CF_s \ ; \qquad \text{(Eq. 4.2)}$$

Here, m_s is the output mass of a given life cycle process categorized under economic sector s, and CF_s is the work environment characterization factor for economic sector s. Calculation of CF_s is performed by using Eq. 4.3:

$$CF_s = \frac{\sum_s Y_s}{\sum_s M_s} \ ; \qquad \text{(Eq. 4.3)}$$

Here, Y_s is the disability adjusted life years (DALY) for economic sector s, and M_s is the total output of economic sector s.

4.1.3.3. LCIT method

LCIT method results are calculated by using Eq. 4.4:

$$Impact\ Score\ LCIT = \sum_i m_i EF_i \ ; \qquad \text{(Eq. 4.4)}$$

Here, m_i is the mass of intermediate flow substance i, and EF_i is the effect factor (disease cases/kg intake) of substance i. EF_i is calculated by the USEtox model (USEtox, 2017).

4.1.3.4. Modified LCIT method

The modified LCIT method assumes that 0.19% of each volatile or gaseous intermediate flow substance will be emitted into the environment, and calculates the impacts by using the same equations as the Simplified LCA.

4.1.3.5. Usage and emission amounts

DNELs or similar ‘no effect’ or ‘lowest observed effect values’ values cannot be used to derive the dose-response slope for toxicity. Hence, reprotoxicity and endocrine disruption effects need EC50 values for dose-response slope calculation of these effects. However, studies on reprotoxicity and endocrine disruption usually focus on finding out the ‘no effect’ values or the ‘lowest observed effect values’ (Chemsafetypro, 2019a). Due to this limitation, the evaluation of SVHC substances (except for carcinogenic or mutagenic ones) was done based on qualitative data, such as the degree of certainty (e.g., ‘suspected reprotoxicity’, ‘reprotoxic animal studies’, ‘known reprotoxic’, etc.), usage and emission amounts.

The carcinogenicity and mutagenicity of substances is usually positively correlated; hence, the method assumes that the mutagenic impacts can often be represented by the carcinogenic impacts of substances (Chemsafetypro, 2019b). Yet, this approach might exclude mutagens with no carcinogenic effects. The equation for the calculation of usage amounts along the life cycle is given in Eq. 4.5:

$$U(h) = \sum_p m_{h,p} \ ; \qquad \text{(Eq. 4.5)}$$

Here, m is the mass of an intermediate substance flow normalized to the functional unit, h is the hazard category (e.g., a suspected carcinogen), and p is the processes along the life cycle.

4.1.3.6. Risk assessment

Use of ECETOC TRA was proposed to calculate RCRs for different AoP. RCRs are simply the ratio of the predicted exposure to the safe exposure levels. The predicted exposures are estimated by ECETOC TRA software as predicted environmental concentration (PEC) for environment or as exposure levels for humans. The software uses generic release values (based on PROcess Categories (PROCs) and Environmental Release Categories (ERCs)) for each activity/product type and calculates exposure values to workers/consumers and environmental concentrations. Recently, ECETOC TRA can address consumer exposures originating only from mixtures, but not from articles. Environmental concentrations are calculated based on Level III (steady state) multimedia fugacity model (ECETOC, 1994). Safe exposure levels can be expressed as predicted no effect concentration (PNEC) for environment and derived no effect levels (DNELs) for humans (ECETOC, 2014; ECETOC, 1994). DNELs are usually derived from animal toxicity studies, especially mice as a small mammal, by extrapolation based on metabolism rate and body weight, and by using the precautionary principle. These values, and all the necessary data for risk assessment (except for PROCs and ERCs), can be found on ECHA's website. PROCs and ERCs can be found in the 2015 ECHA guidance report (ECHA, 2015). Long-term toxicity values were considered as the effects can be observed at lower concentrations. As no safe exposure threshold value exists, for PBTs/vPvBs, no RCRs can be calculated. The same is true for non-threshold CMRs. However, for non-threshold CMRs derived maximum exposure levels (DMELs) based on acceptable risk might be present and can be used if DNELs are not available.

The risk characterization ratios are derived by using Eq. 4.6 and Eq. 4.7.

$$RCR_{environment,c} = \frac{PEC_c}{PNEC_c}; \qquad \text{(Eq. 4.6)}$$

Here, PEC is the predicted environmental concentration in compartment c, and PNEC is the predicted no effect concentration for organisms in compartment c.

$$RCR_h = \frac{Exposure_h}{DNEL_h}; \qquad \text{(Eq. 4.7)}$$

Here, *DNEL* is the derived no effect level for human category h (worker or consumer).

4.1.4. Evaluation of the results

Evaluation of the environmental impact assessment results is not straightforward due to the lack of the cause-effect chain for some hazard categories. RA and usage/emission amount results that could not be converted into DALY or species.yr units are difficult to integrate. Hence, the outcome of RA and usage/emission amounts and the rest of the methods should be used based on the goal of the assessor. Evaluation of the results will be done as described in Section 2.6.

4.1.5. Implementation

The selected alternative will be adopted by the company step by step to derive the technical aspects of an extensive adoption, eventually expanding the adoption of the alternative to all the relevant processes. After the substitution, the company should also keep an eye on the possible improvements in the future.

4.1.6. Detailed explanation of the part of the proposed environmental impact assessment model concerning life cycle stages

Explanation of the application of the Simplified LCA, WE-CFs, LCIT, Modified LCIT methods (except for the usage amounts method) as a part of the proposed environmental impact assessment model is given below (see also Fig. 4.3). These methods include life cycle thinking unlike local assessment methods, such as the risk assessment and emission amounts method.

In general, the scope of the LCA method should be defined at the beginning of the assessment, and, after the initial inventory analyses, the scope might need to be updated. The scope must be defined for the system boundaries (whichever 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 the Simplified LCA (as will be used in this thesis), the scope will be ‘from cradle to gate’ for intermediate-producers, and ‘from cradle to grave’ for end-producers. Here, an ‘intermediate-producer’ is any producer that sells their defined product/service to another industrial producer. An ‘end-producer’ is any producer that sells their defined product/service to consumers.

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

Inventory Analysis: LCI for the Simplified LCA can be formed by using only the input-output analysis data from the company, including direct emissions, and in the case of end-producers, some extra data for the use phase input-output and waste treatment type. The general scope for the ‘cradle to grave’ LCA and the information needed for the Simplified LCA part of the proposed environmental impact assessment model is shown in Fig. 4.4.

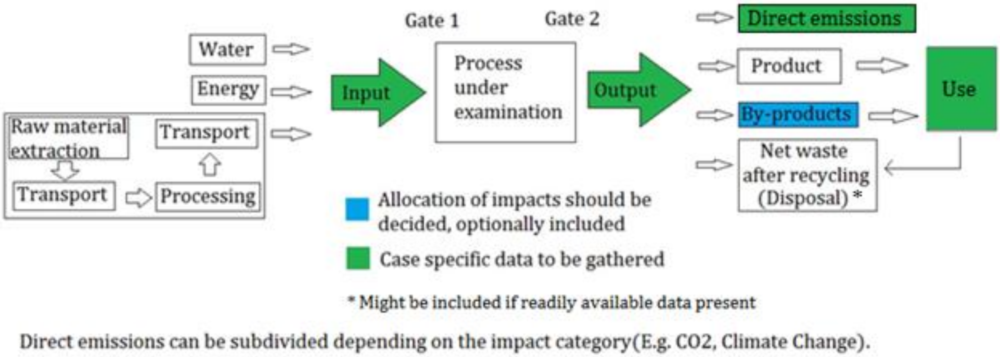

Fig. 4.4. Life cycle stages simplified diagram of the scope for end-producer and data to be obtained (the use phase should be considered only if the product has been changed in any aspect after the substitution)

Generally, in cases where some part of LCI (e.g., a missing chemical and hence the life cycle data related to the missing chemical) cannot be found in the LCI database according to the ILCD handbook (EU, 2010a), 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. The USEtox methodology is a well-known tool that is being used for this purpose. In neither situation will there be a direct collection of data beyond the defined scope of the LCA method (but if there is already available data, it can be used). The industry average data will be used from LCI databases (e.g., Ecoinvent).

A step-by-step flowchart guide for the implementation of the life cycle components of the proposed environmental impact assessment model is presented (see Fig. 4.3):

Step 1 to Step 13 will be performed by the general guidance established by the Institute for Environment and Sustainability in the European Commission Joint Research Centre (EU, 2010a). Fig. 4.3 explains the main steps. Step 3 and Step 4 use the scope and process input/output for the target product/service, respectively. This data can be obtained from the initial assessment as described in Section 4.1.1.

Apart from the traditional approaches, the 'wisdom of the crowds' effect can potentially be used to approximate the supply chain impacts of an unknown process by using 'mistakes' around this 'correct' (but missing) process, as explained in Section 4.2.

In *Step 14*, we run the process network analysis in Simapro software separately for the baseline and the alternatives scenario. For each case, we adjust the cut-off for 'airborne emissions' of CO_2 (carbon dioxide, fossil) for the 'inventory' until at least 40–50 processes are left (excluding 'market processes'), and obtain the outputs of each process. CO_2 (fossil) cut-off is being used because of the potential of CO_2 (fossil) emissions to reflect energy consumption due to a wide use of fuels with the fossil origin (British Petroleum [BP], 2018). Energy consumption is proved to be proportional to the environmental impacts in most cases (Huijbregts *et al.*, 2010; Huijbregts *et al.*, 2006). This is considered to be due to the fact that energy consumption is usually proportional to the number of products produced, activities or the amount of transport distance taken, etc. Due to the statistical effect mentioned in Section 4.2, random variations of toxicity, exposure, etc. tend to approach to a mean when a very high number of processes is considered. Based on this fact, it can be assumed that the energy consumption will be proportional with the worker impacts as well when the whole life cycle of a product is considered. The number of representative processes (i.e., at least 40–50) was determined according to the results obtained in Section 4.3.1. As covering more processes increases the accuracy of the assessment, assessors should consider including more processes if there is enough time and resources to perform the assessment. Hence, adjusting cut-off for 'airborne emissions' of CO_2 (carbon dioxide, fossil) for the 'inventory' until at least 40–50 processes (excluding 'market processes') are left theoretically, in most cases, should cover the most impactful processes.

In *Step 15*, the NACE Rev. 2 categorization of the economic activities should be done. The outputs of each NACE Rev. 2 activity can be calculated for the EU and readily presented to the assessor.

In *Step 16*, the DALYs for each NACE Rev. 2 activity can be readily provided to the assessors (see Annex I for the derivation of these DALYs). Here, the assumption is that the involved processes may be thought to involve occupational safety risk as in Europe (EU-28).

In *Step 17*, the outputs of each process obtained in Step 14 are multiplied with the corresponding WE_DALYs from Step 16 according to its classification as defined in Step 15. We take the sum of the results over all NACE Rev. 2 activities.

In *Step 18*, human cancer/non-cancer effect factors are derived for intermediate organic chemicals that are the outputs of the determined processes in Step 14 by using USEtox software (USEtox 2.1 is being used in this study, and the emission compartment is set to 'Emissions to industrial indoor air' in 'Industry, OECD' area).

In *Step 21*, all intermediate chemicals are entered, as defined in Step 14, into SimaPro software as 'emissions to air (low population, long term)' for chemicals with high volatility (i.e., with vapor pressure 0.01 kPa or more at room temperature (IPPC, 2010)) and 'emissions to water (unspecified)' for the rest of the chemicals. We run impact assessment by employing the ReCiPe Endpoint (E) methodology and obtain the endpoint impact scores for 'emissions to air' and 'emissions to water' separately.

In *Step 23*, the results of the modified LCIT method (Step 21) for 'emissions to air' can be made compatible with simplified LCA results if we know the fugitive and accidental emission amounts. The data existing in the literature is applicable for the fossil fuel industry (IPCC, 2006). Natural gas is mostly methane, with approximately 90% of Danish gas (Plejdrup, Nielsen and Nielsen, 2015). Fugitive (including accidental) methane emissions from gas production (gas flaring excluded) were assumed to be applicable to fugitive (and accidental) emissions of high volatility chemicals and gases as this was the only comprehensive data available. For developed countries, methane emissions of 1.34E-3 (average of 3.80E-4 and 2.30E-3) Gg per 10^6 m^3 of produced gas were adopted. This corresponds to approximately 0.19% overall loss of natural gas, when adjusted for the assumption of 90% methane representing 100% of the natural gas, and unit conversions were conducted (WNA, 2016; IGU, 2012). Another study in 2009 by the Environment Accounts and Statistics Division reported gasoline (a high volatility mixture) evaporative losses of approximately 0.14% to 0.17% in such a relatively cold country as Canada (Environment Accounts and Statistics Division, 2012). The study also stressed the research needs in this area regarding whether or not these loss amounts are applicable to other industries and pollutants (Environment Accounts and Statistics Division, 2012). Hence, due to lack of more detailed comprehensive data, the 0.19% loss will be used for the purposes of this thesis, and the modified LCIT results for high volatility chemicals (with a vapor pressure of more than 0.01 kPa at room temperature) and gases should be multiplied with 1.90E-3 and added to the simplified LCA results for each endpoint impact category.

Also, the results of the LCIT method can be made compatible by applying a factor of 1.3E-5 DALY/cancer disease case, and 3E-6 DALY/non-cancer disease case, as derived in Section 2.6.

The use of the Europe ReCiPe Endpoint (E/A) normalization factors and weightings was adopted to further simplify the scores from Step 13, Step 21 and Step 22. The normalization factors are as follows: 24.3 (human health), 3,640 (ecosystems) and 0.00324 (resources). The weightings are as follows: 400 (human health), 400 (ecosystems) and 200 (resources).

As the remaining results from the ‘modified LCIT method’ (such as the modified LCIT results for less volatile chemicals) are not comparable with the simplified LCA scores or with the WE-CFs results, the remaining results from Step 21 should be evaluated independently with personal or group judgement.

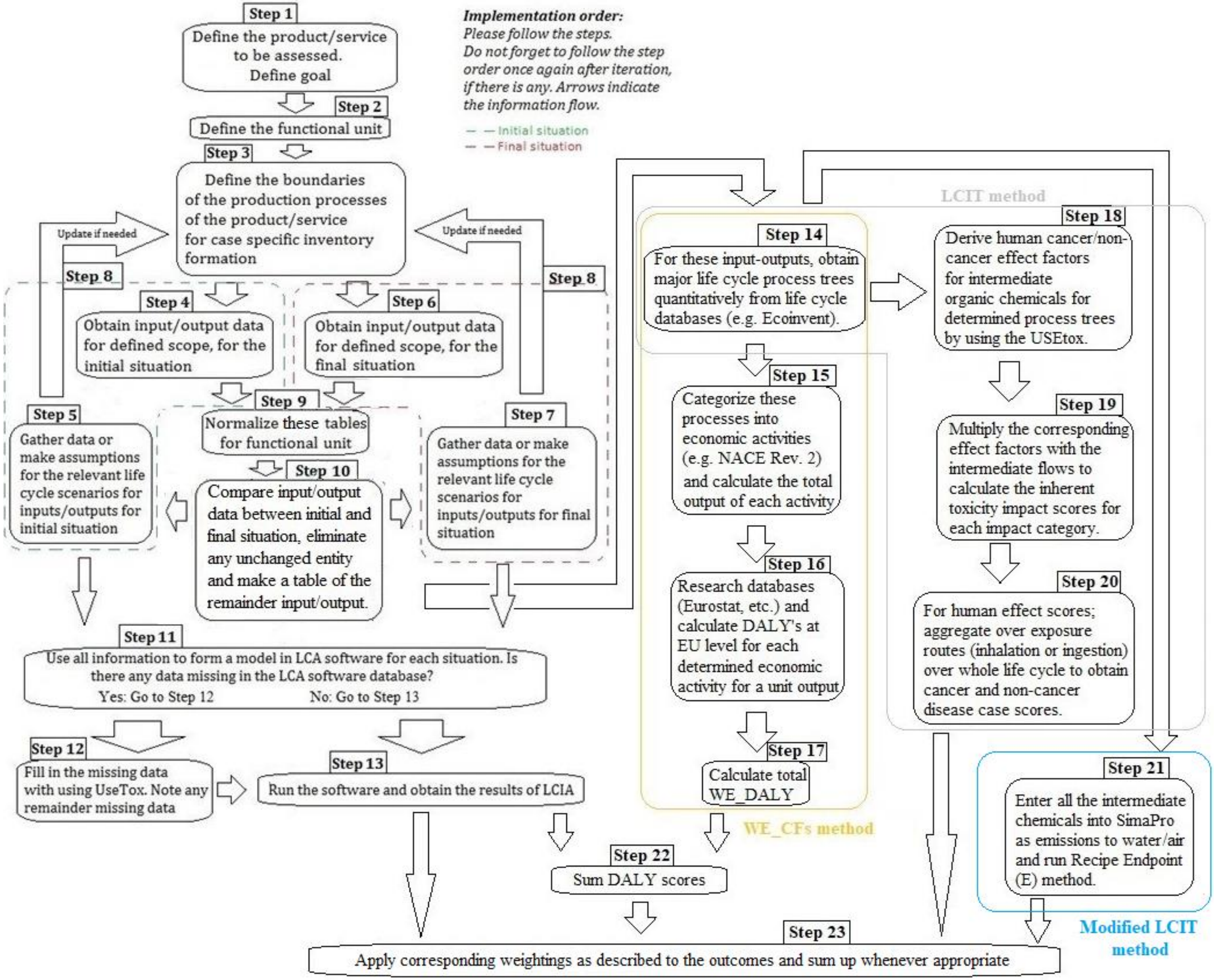

Fig. 4.3. A more detailed flowchart explanation of simplified LCA, WE-CFs, LCIT and Modified LCIT methods as part of the proposed thesis model for environmental impact assessment

4.2. Proposed methodology for the examination of the ‘wisdom of the crowds’ effect

A qualitative way for the determination of the existence of the ‘wisdom of the crowds’ effect (see Section 4.3.3 for detailed explanation) was proposed to evaluate the areas of further research in addition to the proposed quantitative examination which will be outlined shortly. According to the proposed qualitative methodology, the existence of the ‘wisdom of the crowds’ effect for a given entity can be evaluated by analyzing the entities with regards to the existence of error probability distributions around a correct value (including cut-off distributions), ‘sufficient’ number of independent random selections from these distributions, and aggregation over these independent selections (see Table 5.55 in Section 5.4.1). The questions to be asked are: “Is the correct value always the most likely outcome (mode) of the distribution and is the distribution non-uniform?”, “Does the correct value (mode) of the (inexpert) distribution among all possible distributions have a biased position in the distribution (e.g., is it always skewed to the left)?” (as in Fig. 4.5) and “Is there any aggregation of these individual decisions being performed?”. The non-uniform distributions were assumed to resemble (even partly) the normal or lognormal distribution. Physical measurements with devices that feature many degrees of freedom (many potential errors) tend to yield normal distributions due to the ‘central limit theorem’ (Petrov, 1995). Hence inventory measurements are expected to deliver a normal distribution if the errors are relatively small when compared to the correct measurement value. However, if the errors are large, the distribution is expected to be skewed as the errors reach a boundary (e.g., negative mass is not possible). Under such circumstances, the errors rather resemble a lognormal distribution (Qin, Suh, 2017). Hence LCI amounts can be assumed to show such distributions. Similarly, the central limit theorem can be used to stress that the errors in the ‘functional unit’, ‘reference flow’, ‘inventory amount’, ‘effect factors’ and ‘intermediate flows’ would be normally distributed when relatively small errors are being considered, and, for large errors, the lognormal distribution would be more realistic. Hence, the shape of the error distribution also depends on the expertise of the assessors or the accuracy of the measurement tool. ‘Obtaining data’ is assumed to have a systemic bias as inexpert assessors tend to ignore any unknown data; hence the mode of the distribution does not always coincide with the correct value. The type of the distribution affects the accuracy of the ‘wisdom of the crowds’ effect, and this assumption needs to be examined quantitatively afterwards. In the second question, the mode of the distribution can be biased for two reasons: bias of the inexpert assessor or the bias in the system itself.

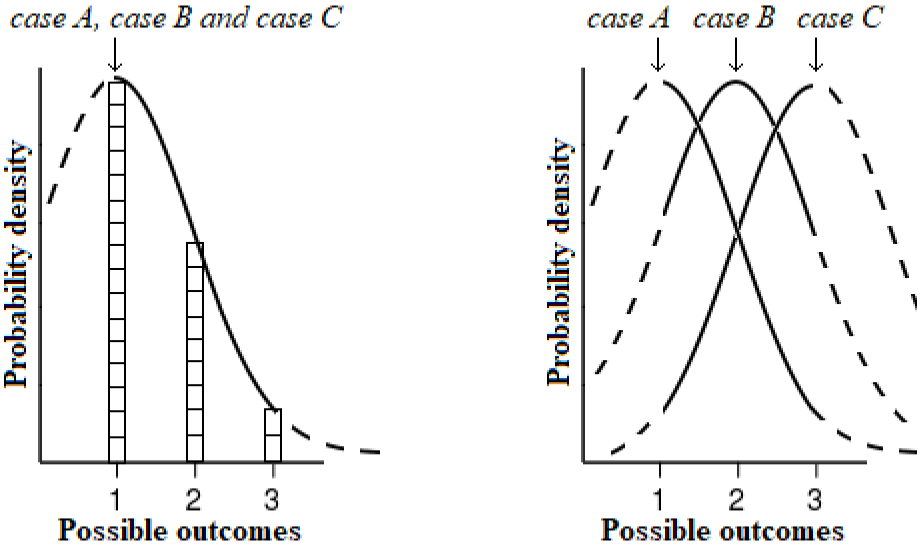

Fig. 4.5. Visual aid for answering the question "Does the correct value (mode) of the (inexpert) distribution among all possible distributions have a biased position in the distribution?". Bias of the inexpert assessor towards 'outcome 1' is demonstrated on the left. Probability distributions for an (almost) expert assessor are demonstrated on the right for a non-biased system. In the case of the bias in the system itself, the mode would be biased even for the (almost) expert assessor. Discrete distributions are represented by nearby segments of continuous distributions

Quantitative examination of the 'wisdom of the crowds effect' in simplified life cycle assessments (Simplified LCAs) was proposed and performed by using four cases of solvent-based paint (Table 4.2 outlines the company input-output data). The correct input-output values were modified independently 40 times to create error cases. In each of these cases, the (simulated) assessors were assumed to have limited knowledge and to make random mistakes based on their knowledge. The mistakes considered for Case 1 (Metal sheet priming baseline situation, expert case), Case 2 (Metal sheet priming alternative situation, expert case) and Case 4 are: confusion of the solvent type (e.g., Xylene instead of Isopropanol), similar sounding chemicals (e.g., Benzene instead of Ethyl benzene), general air emission types (e.g., a volatile organic compound (VOC) or a non-methane volatile organic compound (NMVOC) instead of a specific organic chemical), the origin of country or region, and the technology type. In Case 3, the assessor was assumed to be more knowledgeable and confused only similar sounding chemicals (e.g., Butyl acetate or Ethyl benzene instead of Ethyl acetate), the origin of country or region, and the technology type. All inexpert assessors chose consequential system modelling as inventory modelling and entered the inventory amounts correctly.

The results are obtained for the Recipe Endpoint characterization and damage impact methodologies. The obtained results were averaged (arithmetic and geometric averages) for various numbers of inexpert assessors (propagation from 1 to 40) and compared to the correct result as the percentage error.

Table 4.2. Company input-output data of solvent-based paints

	Inventory for Case 1 (kg)	**Inventory for Case 2 (kg)**	**Inventory for Case 3 (kg)**	**Inventory for Case 4 (kg)**
Inputs	*Dipropylene glycol monomethyl ether (1474)*	*Isopropanol (1474)*	*Ethyl acetate (40)*	*Xylene (50)*
	Xylene (1474)	*Toluene (1474)*	*Isopropanol (8)*	*Propane (25)*
	Ethyl benzene (295)	*Xylene (555)*	*Butyl acetate (33)*	*Butane (10)*
	*Lorry 7.5-16 t EURO3 (5522 t*km)*	*Ethylbenzene (174)*		*Naphtha (10)*
	Heat, small-scale, natural gas [EU without CH), at boiler atmospheric non-modulating <100kW (1254 MJ)	*Naphtha (208)*		
		*Lorry 7.5-16 t EURO3 (6605 t*km)*		
Air emissions	*Propylene glycol monoethyl ether (1474)*	*Isopropanol (1474)*		
	Xylene (1474)	*Toluene (1474)*		
	BTEX (Benzene, Toluene, Ethylbenzene, and Xylene), unspecified ratio (295)	*Xylene (555)*		
		NMVOC (174)		
		Naphtha (208)		

4.3. Statistical methods and findings to be used in model development

Various statistical phenomena from different studies were adopted for the application of the proposed environmental impact assessment model. These phenomena are as follows: sampling for the purpose of determination of the complete set distribution, proportionality of the environmental impacts with the energy usage, and the ‘wisdom of the crowds’ effect.

4.3.1. Analyzing LCI databases for the determination of the optimum number of representative processes

Selection of representative processes was necessary due to time and resource limitations. Representative processes were selected to represent the supply chain of the products in calculation of their environmental and occupational impacts.

The Ecoinvent Version 3 LCI database was analyzed to determine an optimum number of representative processes that can be used for impact assessment (Ecoinvent, 2017). As life cycle relative risk assessment methods are not yet readily automated – and are thus manually performed, it was necessary to carry out this analysis in order to be able to apply subsequent methods that are proposed in this thesis for the risk assessment of accidents considering workers’ safety (WE-CFs method) and for relative risk assessment considering workers' health (the modified LCIT method) and environmental health (the modified LCIT method).

The LCI database was examined for the percentage contribution of the top positions contributing 10, 20 and 40 major processes to climate change (kg CO_2 equivalent) for a given process network by using SimaPro 8.5.2.0 Analyst software and ReCiPe Midpoint (E) V1.13, Europe, characterization step yet excluding infrastructure processes. The 'Process networks' in the Ecoinvent Version 3 database recently included 6,277 processes, and the validity of the representative quality of selecting a few (e.g., 40) processes had to be justified. 'Process networks' were selected randomly from the Ecoinvent Version 3 LCI database (Ecoinvent, 2017). For each selected process network, direct or indirect 'process contribution' for climate change (CO_2 equivalent emissions) was analyzed, and the results were noted as in Table 4.3.

Table 4.3. Process contributions to climate change impacts (CO_2 equivalent emissions). Contribution values below 75% are written in italic and bold.

Characterization/Climate change/CO_2 equivalent **(ReCiPe Midpoint (E) V1.13/ Europe ReCiPe (E))** **Database: Ecoinvent 3**	**Top 10 processes**	**Top 20 processes**	**Top 40 processes**	**Top 60 processes**	**Top 80 processes**	**Top 100 processes**	**Total number of nodes**
Titanium dioxide {RoW}| production, sulfate process | Conseq, U	116%	110%	112%	109%	105%	104%	6037
Alkylbenzene, linear {RoW}| production | Conseq, U	106%	109%	107%	105%	103%	102%	6038
1-pentanol {RoW}| hydroformylation of butene | Conseq, U	103%	108%	106%	107%	104%	97%	6037
Isopropanol {RER}| production | Conseq, U	93%	101%	101%	101%	103%	100.3%	6037
Isopropanol {RoW}| production | Conseq, U	98%	100.4%	101%	102%	101%	101%	6037
Transport, freight, lorry 7.5-16 metric tons, EURO4 {RoW}| transport | Conseq, U	97%	99%	100.3%	100.2%	100.2%	100%	6038
Acetone, liquid {RER}| production | Conseq, U	100%	100%	100%	100%	100%	100%	6037
Acetone, liquid {RoW}| production | Conseq, U	100%	100%	100%	100%	100%	100%	6037
Electricity, high voltage {RoW}| electricity production, oil | Conseq, U	99%	100%	100%	100%	100%	100%	6037
Sodium percarbonate, powder {GLO}| market for | Conseq, U	99%	100%	100%	100%	100%	100%	6037
Toluene, liquid {RER}| production | Conseq, U	99.9%	100%	100%	100%	100%	100%	6037
Toluene, liquid {RoW}| production | Conseq, U	99.9%	100%	100%	100%	100%	100%	6037
Xylene {RER}| production | Conseq, U	99.9%	100%	100%	100%	100%	100%	6037
Xylene {RoW}| production | Conseq, U	99.9%	100%	100%	100%	100%	100%	6037
Alkylbenzene, linear {RER}| production | Conseq, U	79%	93%	99%	99%	100%	101%	6038
Electricity, high voltage {RoW}| electricity production, hydro, reservoir, alpine region | Conseq, U	97%	99%	99%	99.6%	99.8%	100%	6037
Sulfur hexafluoride, liquid {RER}| production | Conseq, U	98%	99%	99%	99%	99.5%	99.6%	6037
Transport, freight, lorry 7.5-16 metric tons, EURO4 {RER}| transport | Conseq, U	95%	98%	99%	99%	99.8%	99.8%	6038
Electricity, high voltage {RoW}| electricity production, wind, >3MW turbine, onshore | Conseq, U	91%	95%	98%	99%	99%	99.7%	6037
Sulfur hexafluoride, liquid {RoW}| production | Conseq, U	96%	97%	98%	99%	99%	99.6%	6037
Ethyl benzene {RER}| production | Conseq, U	93%	96%	97%	98%	98%	99%	6037
Hard coal briquettes {RER}| production | Conseq, U	83%	92%	97%	98%	99%	99%	6038

Characterization/Climate change/CO_2 equivalent **(ReCiPe Midpoint (E) V1.13/ Europe ReCiPe (E))** **Database: Ecoinvent 3**	**Top 10 processes**	**Top 20 processes**	**Top 40 processes**	**Top 60 processes**	**Top 80 processes**	**Top 100 processes**	**Total number of nodes**
Nitrogen fertilizer, as N {RoW}| urea ammonium nitrate production | Conseq, U	91%	94%	97%	97%	98%	99%	6037
Refrigerant R134a {RoW}| production | Conseq, U	96%	97%	97%	98%	99%	99%	6037
Urea formaldehyde resin {RoW}| production | Conseq, U	90%	94%	97%	98%	99%	102%	6037
Ethyl benzene {RoW}| production | Conseq, U	94%	96%	96%	98%	99%	99%	6037
Hard coal briquettes {RoW}| production | Conseq, U	86%	92%	96%	98%	99%	99%	6038
Refrigerant R134a {RER}| production | Conseq, U	92%	94%	96%	97%	98%	98%	6037
Nitrogen fertilizer, as N {RER}| urea ammonium nitrate production | Conseq, U	90%	91%	95%	97%	98%	98%	6037
Acetoacetic acid {RER}| production | Conseq, U	***74%***	89%	94%	97%	99%	99%	6038
Clay brick {RER}| production | Conseq, U	89%	91%	94%	96%	97%	98%	6037
Acetoacetic acid {RoW}| production | Conseq, U	81%	87%	93%	94%	95%	96%	6038
Clay brick {RER}| production | Alloc Def, U	86%	89%	93%	95%	96%	97%	9641
3-methyl-1-butyl acetate {RER}| production | Conseq, U	***62%***	83%	91%	95%	97%	99%	6041
Clay brick {GLO}| market for | Conseq, U	82%	87%	91%	94%	96%	97%	6037
Titanium dioxide {RER}| production, sulfate process | Conseq, U	85%	79%	91%	92%	93%	96%	6037
Transport, pipeline, onshore, petroleum {RER}| processing | Conseq, U	***56%***	81%	91%	93%	96%	97%	6037
Ammonium carbonate {RER}| production | Conseq, U	***62%***	77%	90%	92%	94%	96%	6037
1-pentanol {RER}| hydroformylation of butene | Conseq, U	***72%***	82%	88%	94%	96%	96%	6037
2-methyl-1-butanol {RER}| hydroformylation of butene | Conseq, U	***72%***	82%	88%	94%	96%	96%	6038
Ammonium carbonate {RoW}| production | Conseq, U	76%	85%	87%	91%	95%	97%	6037
Clay brick {GLO}| market for | Alloc Def, U	76%	82%	87%	90%	92%	94%	9641
Sulfuric acid {RER}| production | Conseq, U	***47%***	***69%***	87%	93%	95%	97%	6037
Alkyd paint, white, without solvent, in 60% solution state {RER}| production | Conseq, U	***52%***	78%	85%	88%	92%	93%	6037
Alkyd paint, white, without solvent, in 60% solution state {RoW}| production | Conseq, U	***60%***	75%	85%	89%	92%	94%	6037
Steel, low-alloyed, hot rolled {RER}| production | Conseq, U	***56%***	***73%***	82%	88%	92%	94%	6037

Characterization/Climate change/CO$_2$ equivalent **(ReCiPe Midpoint (E) V1.13/ Europe ReCiPe (E))** **Database: Ecoinvent 3**	**Top 10 processes**	**Top 20 processes**	**Top 40 processes**	**Top 60 processes**	**Top 80 processes**	**Top 100 processes**	**Total number of nodes**
Steel, low-alloyed, hot rolled {RoW}| production | Conseq, U	***57%***	***73%***	82%	88%	92%	94%	6037
Acetyl chloride {RER}| production | Conseq, U	***53%***	***65%***	81%	87%	91%	92%	6038
Titanium dioxide {RoW}| production, sulfate process | Alloc Def, U	***64%***	***71%***	80%	84%	88%	90%	9641
Acrylic varnish, without water, in 87.5% solution state {RoW}| production | Conseq, U	***48%***	***64%***	78%	85%	88%	92%	6037
Transport, pipeline, onshore, petroleum {RoW}| processing | Conseq, U	***48%***	***57%***	78%	88%	94%	96%	6037
Ethylene glycol dimethyl ether {RoW}| production | Conseq, U	***59%***	***72%***	77%	81%	87%	91%	6038
Alkyd paint, white, without solvent, in 60% solution state {RoW}| production | Alloc Def, U	***54%***	***65%***	75%	81%	85%	88%	9641
Acrylic varnish, without water, in 87.5% solution state {RER}| production | Conseq, U	***46%***	***63%***	***74%***	81%	85%	90%	6037
Ethylene glycol dimethyl ether {RER}| production | Conseq, U	***56%***	***60%***	***74%***	80%	87%	90%	6038
Alkyd paint, white, without solvent, in 60% solution state {RER}| production | Alloc Def, U	***54%***	***63%***	***72%***	77%	81%	84%	9641
Impact extrusion of aluminum, 1 stroke {GLO}| market for | Conseq, U	***39%***	***56%***	***72%***	79%	84%	88%	6061
Impact extrusion of aluminum, 1 stroke {RER}| processing | Conseq, U	***39%***	***56%***	***72%***	79%	84%	88%	6059
Sulfuric acid {RoW}| production | Conseq, U	***44%***	***51%***	***72%***	83%	90%	94%	6037
Glyphosate {RoW}| production | Conseq, U	***40%***	***55%***	***71%***	79%	84%	88%	6037
Titanium dioxide {RER}| production, sulfate process | Alloc Def, U	***53%***	***62%***	***71%***	78%	82%	85%	9641
Glyphosate {RER}| production | Conseq, U	***31%***	***43%***	***61%***	***71%***	80%	85%	6037
Impact extrusion of aluminum, 1 stroke {GLO}| market for | Alloc Def, U	***27%***	***38%***	***56%***	***66%***	***73%***	78%	9653
Impact extrusion of aluminum, 1 stroke {RER}| processing | Alloc Def, U	***27%***	***38%***	***56%***	***66%***	***73%***	78%	9651

In total, 64 processes were chosen; 56 processes with consequential modelling and 8 processes with allocation modelling were randomly chosen from different sectors. Among 34 of those processes, Top 10 was enough to represent over 75% of the emissions. In 8 processes, Top 20 was enough to represent over 75% of the emissions. In 7 processes, Top 40 was enough to represent 75% of the emissions, and only 6 processes needed to include Top 60 to represent over 75% of the emissions. Consequential modelling performed better in this aspect due to fewer nodes (usually 6,037 compared to 9,641; markets included) and the system expansion/substitution, as, usually, negative emissions tend to dramatically oppose positive emissions from low emission processes along the life cycle. For the same reason, some percentages were higher than 100%. This phenomenon was so prominent that for the process 'Titanium dioxide {RER}| production, sulfate process | Conseq, U', Top 10 processes were a better representative than the Top 20 processes as negative emission processes caused by system expansion/substitution were comparable in magnitude to the processes with positive emissions.

Some processes could be represented with very few (fewer than 10) processes. The 'Toluene, liquid | production | Conseq, U' process and the 'Xylene | production | Conseq, U' process were among such processes. With toluene being a cheap by-product of petroleum refinery operations, a very minor part of impacts attributed to it by 'economic attribution' and virtually all of its upstream impacts can be neglected and attributed to other high price products resulting from petroleum refinery. 'Transport, freight, lorry 7.5–16 metric tons, EURO4 {RER}| transport | Conseq, U' was another process of this type that could be represented by a few processes, but this was due to the exclusion of infrastructure processes.

According to these findings, it was possible to select relatively few representative processes for most products. Hence, the 'Network' option of SimaPro 8.5.2.0 Analyst can be used to find the representative processes. The cut-off with the 'Network' option differs from the cut-off with the 'Process contribution' option, as, in the 'Network' option, the downstream processes connected to the major fossil CO_2 emitting processes (i.e., energy consumption) were shown as well. This was desirable as we can thus assume that the processes which are downstream to the major energy consuming processes are also expected to have high environmental and occupational impacts. Such processes, although not being major fossil CO_2 emitters within their gate-to-gate boundaries, indirectly use the majority of the energy and/or materials produced in the major upstream processes.

4.3.2.Examination of ‘inexpert outcome’ for systematic errors in Simplified LCA

Selected impact assessment module for ‘inexpert outcome’ systematic error evaluation

The LCA part of the impact assessment model is selected for the application of ‘inexpert outcome’ examination.

Random/systematic assessor mistakes

Assessors will be considered to correctly know the chemical names and amounts, also, they are assumed to be able to correctly choose ‘market for, Conseq, U’. Based on this, the maximum number of mistakes will be assumed, and LCA will be performed for the case with the maximum number of mistakes involving at least one systematic error per case.

Comparison of the outcomes

The outcomes will be compared with the following formula (Eq. 4.8):

$$\%_i = 100 \times \left(\frac{Non\ expert - Expert}{Expert}\right)_i ; \qquad \text{(Eq. 4.8)}$$

Here, i is the case number.

4.3.3.Theoretical examination of the practical value of the proposed thesis model for impact assessment from the random error point of view

Inexpert assessor randomly choosing from sets of life cycle process inventories

There are three sets of conditions that give rise to the phenomenon of the ‘wisdom of the crowds’: existence of error probability distributions around a mean that is not determined by a systematic error, ‘sufficient’ number of independent random selections from these distributions, and aggregation over these independent selections (refer to Fig. 4.8). In terms of probability distributions, this study assumes a Gaussian (normal) or lognormal distribution set to explain this effect. This phenomenon is known to be valid for Gaussian, log-normal and hybrid distribution sets (Gaussian and log-normal mixed in a set of distributions) (Hawkins, 1991). The validity of this phenomenon for other types of distribution sets was not included in the current study and can be a further research area for the investigation of this effect with different distribution types of databases/inventories/errors.

In the case of inexpert assessors, surprisingly, the statistical effects are on their side. Such a statistical effect can be simply expressed as: independent random mistakes tend to cancel each other out to some extent. Hence, as long as the assessor is randomly choosing (no systematic error) from a set of inventories with a probability distribution around a ‘correct’ mean, the selection of multiple processes results in a decrease in the total mistake to have been made. The phenomenon can be seen in Fig. 4.6 with the dice roll analogy. The effect of random summation trims the extremes of the total distribution. This phenomenon becomes more dominant as the number of the selected processes increases. The sum of infinite dice rolls is exactly equivalent to the sum of single valued dice (where all sides have the same value) with the value of 3.5 (average of 1 and 6). This is similar to the phenomenon seen in the '*wisdom of the crowds*' effect as well, where the audience makes guesses about a given problem, such as the number of beans in a jar. As the number of guesses increases, the random mistakes cancel each other; hence, the average of the guesses approaches to the mean which is the real number of the beans in the jar. A similar analogy can be made with an inexpert assessor choosing from multiple possible processes for each given process type (e.g., electricity production). This analogy can be seen in Fig. 4.7. Although in Fig. 4.7 the process types are not similar in their inventory distribution, unlike the dice rolls (each dice is exactly the same as any other dice), it can be stressed that the progress towards the mean will still occur as long as the inventories are distributed randomly, and a sufficient amount is considered; hence there is no bias towards any particular direction away from the mean (randomness cannot break symmetry in a large enough sample size).

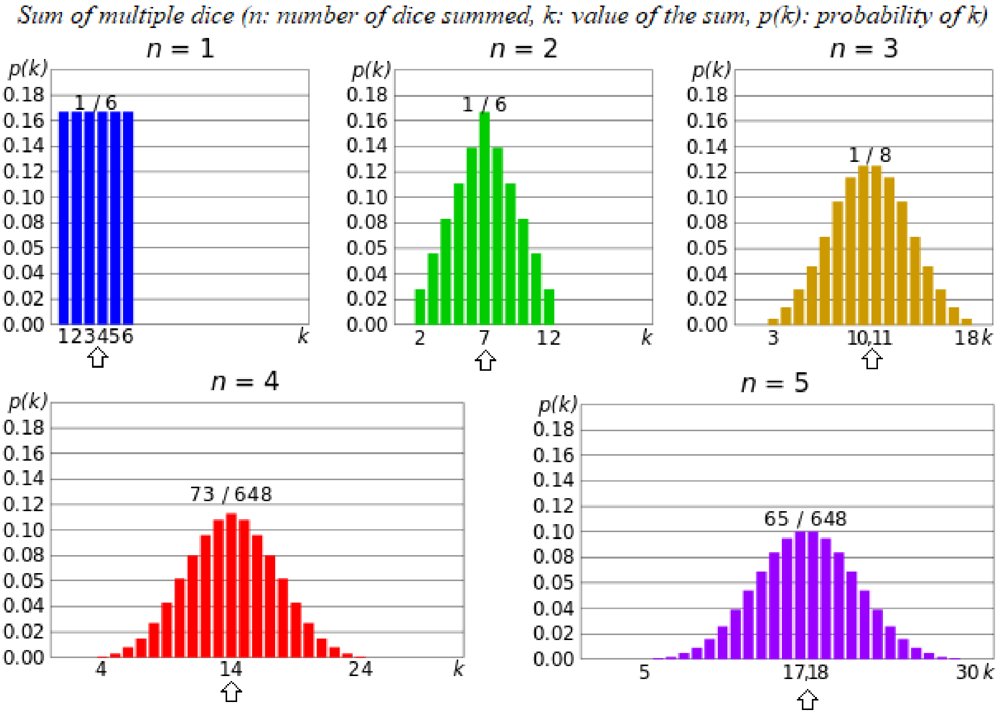

Fig. 4.6. Probability density distributions of the sum of multiple dice; most likely values of the distribution tend to approach the mean. Hence, after infinite rolls, the average dice (k/n, which is the average contribution of a single dice roll to the total sum) has a value of 3.5 [Singh, Dalpatadu and Lucas, 2011]

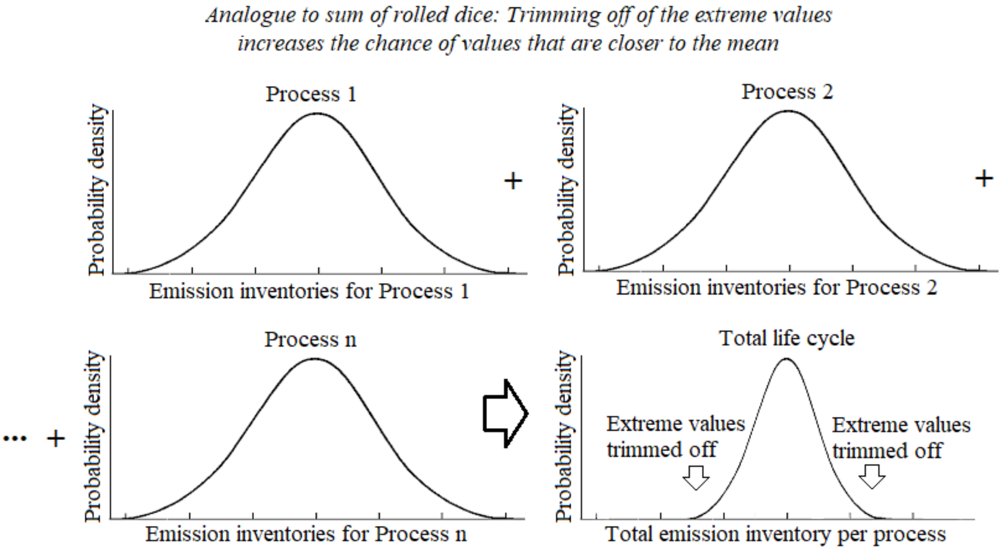

Fig. 4.7. Analogue of dice roll sums; summation over life cycle process inventories. Here, 'Process n' is the process type that the assessor should consider (e.g., electricity production), and 'emission inventories for Process n' are the available inventories for Process n (e.g., electricity production from oil, Hungary)

Hence, the author of the present thesis recognizes that performing assessments with random errors, even if it is done by inexpert assessors, overall might be better than not doing any assessment at all. This realization is important in proposing the application of this statistical effect to the environmental impact assessment methods, whenever expert assessors are limited or unavailable.

For the error distribution for any given assessor, it was assumed that the correct value corresponds to the maximum probability value of the distribution (for Gaussian distributions, the maximum value is equal to the mean). This does not necessarily coincide with the mean value of the distribution. However, the effect still persists if the distributions are independent, and the means of the distributions are randomly distributed, which is another way of saying 'no systematic errors' (as depicted in Fig. 4.8). This is due to the fact that randomness cannot break symmetry in a large enough sample size.

There is another point to be considered: the border effect. The border effect can be described as the cut-off of a probability distribution due to being closer to the borders of the error space (as shown in Fig. 4.8). In the case of a systematic (biased) positioning of the correct values on the error space (that might be caused by the biases of the examined system), the result of the aggregation is expected to approach to a specific point shifted away from the correct aggregated value. However, by using the geometric mean instead of the arithmetic mean, the error can be reduced significantly. This is due to the fact that, for lognormal distributions, the median, which can be approximated by the geometric mean (Limpert, Stahel and Abbt, 2001), is closer to the mode (the assumed correct value) with less distance than the arithmetic mean's distance to the mode.

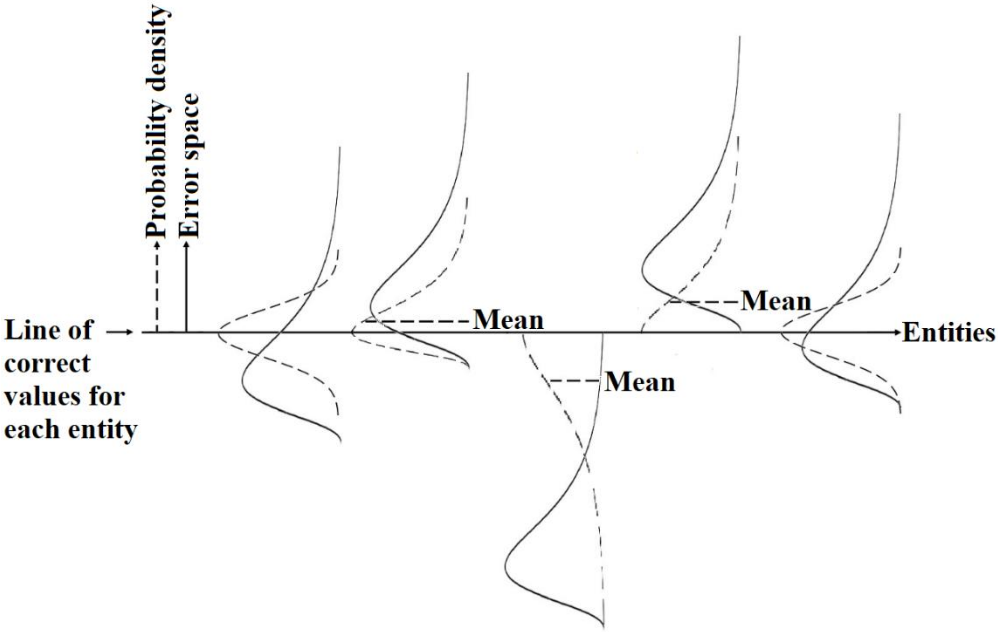

Fig. 4.8. Probability distributions and the 'error spaces' for different entities. The dashed lines represent the probability densities. The continuous lines represent the error space as determined by the total space and the expertise level of the assessor. Probability distributions are not normalized

Sample size requirements

For a given sample set with the same standard deviation (σ_S) and mean (μ_S) values among all the independent n subset individuals in this sample set, the standard deviation of the sum of the n subsets is given by (Easton, McColl, 1997):

$$\sigma = \frac{\sigma_S}{\sqrt{n}} \qquad \text{(Eq. 4.9)}$$

Eq. 4.9 also holds for the sum of the emissions per process over the whole life cycle of a product or the distribution representing the sum of random errors in LCI per process (further data is presented in Annex III). In other words, Eq. 4.9 can be used whenever there is a summation of normal distributions, regardless of the context. If we want to obtain an error that is less than a given value away from the mean of the sum, for a given confidence level, we can write Eq. 4.10:

$$\rho\mu_S \geq z\frac{\sigma_S}{\sqrt{n}}; \qquad \text{(Eq. 4.10)}$$

Here, the left-hand side of Eq. 4.10 is the amount of the margin of error that we want our outcome of the sum to be in, and the right-hand side is the margin of error of the sum for a given confidence level. Here, z represents the critical value for the standard normal distribution (the so-called ‘z-scores’) for a given confidence level (usually taken as 95%, z≈1.96), and ρ is the percent error (away from the mean of the sum) that we tolerate in the sum. If we solve Eq. 4.10 for n, we can write the minimum sample size n_{min} as follows (Eq. 4.11):

$$n_{min} = \left(\frac{z\sigma_S}{\rho\mu_S}\right)^2 \qquad \text{(Eq. 4.11)}$$

In Eq. 4.11, μ_S can be found by dividing the mean of the sum (μ) by the amount of the sample size (n). The mean of the sum (μ) is basically the value that an expert assessor is expected to find. ρ depends on what degree of error we can tolerate in the results, and it can subjectively be taken as 10–15%. The values for σ_S are usually problematic to find, as, commonly, the standard deviation of the samples is not known.

The above equations were derived for the assumption that all the subsets have the same standard deviation (σ_S) and mean (μ_S). In the case where there is also a distribution of σ_S and μ_S, for greater values of n, the estimated standard deviation approaches the standard deviation of the sum, and the estimated mean approaches the real mean of the sum, hence Eq. 4.11 still holds when the average σ_S and μ_S are being used (Yale, 2018). So, the same arguments made above for the distribution of the value of the samples can be made for the distribution of the standard derivation of the samples and for the mean of the samples, hence Eq. 4.11 can be modified based on the standard deviation of these entities.

However, as the standard deviation (σ_S) of any of these entities cannot easily be known for mistakes made by assessors for a given case (although it can be approximated by experimenting with assessors or by analyzing the LCI within the range of possible mistakes by an average inexpert assessor), the sample size effects for a given case cannot be examined by using this approach. Hence, another approach will be taken – as in Section 4.3.2 – by directly examining the percentage error, without being concerned about the standard deviation or the number of independent variables per case. This is the weak point of this approach, specifically, that we do not know the standard deviation per case, nor do we know the size of the possible cases so that we would be able to calculate the statistically meaningful amount of case studies to be examined.

Assumptions: the sample size of the case studies is statistically sufficient. In addition to this, the assumption that an inexpert assessor makes random (non-systematic) mistakes falls apart in certain instances, as the assessors tend to systematically skip chemicals when they fail to find the chemical’s name(s) in the database, hence creating a systematic error towards accounting the impacts less than their real values, which ultimately leads to the underestimation of their impacts. Furthermore, based on the assumptions that the inexpert assessor will correctly know the chemical names and amounts, we are also bound to assume that they will correctly choose ‘market for, Conseq, U’; thus it can be said that the errors an inexpert makes under these circumstances are mostly systematic errors (e.g., ignoring the chemicals that are missing from databases). However, as the ‘wisdom of the crowds’ effect can potentially be used to address these data gaps in life cycle inventories, the effect can still be used to reduce errors and to perform assessments in circumstances whenever assessor resources are limited.

4.4. Description of the expert system (harmonized internet system) for life cycle assessment

‘Consumption products’ are products that are actively consumed regardless of their expected lifetime (e.g., all food products, toilet paper, tooth paste, etc.). ‘Products for use’ are products that are used for a purpose, and which are not actively terminated (e.g., a TV, a fridge, a car, furniture, etc.). ‘Products for use’ are expected to last for their expected lifetime. If this is the case, the expected lifetime (*t*) for the ‘product for use’ will be entered in the HIS-LCA. For consumption products and for all the services, *t* will be set equal to 1.

This question will be asked to the assessor for the ‘products for use’: “One unit of my product can perform ...(*F*)… functional units in 1 year.” This question will be asked to the assessor for the ‘consumption products’ or services: “One unit of my product/service can perform …(*F*)… functional units.”

The open Leontief model will be used as a well-established concept (Obikwere and Ebiefung, 2014) that is being used to link the external demands on the technosphere to the environmental stressors. The model will be used in the proposed expert system for the calculation of the environmental stressors inventory. An input-output matrix (i.e., the requirements matrix) (***A***) as in Eq. 4.12 will be formed by using the data gathered by the harmonized internet system.

$$A = \left[\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & a_{36} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} \\ a_{61} & a_{62} & a_{63} & a_{64} & a_{65} & a_{66} \\ \multicolumn{2}{c}{\underbrace{\hphantom{a_{61}\quad a_{62}}}_{\text{End products/ services}}} & \multicolumn{4}{c}{\underbrace{\hphantom{a_{63}\quad a_{64}\quad a_{65}\quad a_{66}}}_{\text{Intermediate products/services}}} \end{array}\right] \begin{array}{l} \left.\vphantom{\begin{array}{c}0\\0\end{array}}\right\}\text{End products/ services} \\ \left.\vphantom{\begin{array}{c}a\\a\\a\\a\end{array}}\right\}\text{Intermediate products/services} \\ \vphantom{a} \end{array} \qquad \text{(Eq. 4.12)}$$

For alternatives assessment purposes, an external demand matrix (*y*) will be used, such that it will include the demand of every ‘end product/service’ that is linked to the product(s)/service(s) affected by the alternative scenario. However, the end products/services that are positioned on a branch that features a company which declined the alternative scenario will be excluded from this demand matrix. The proposed demand matrix (i.e., the ‘combined total functional demand’) considers the total current demand of consumers for all the relevant functions. This is different from the traditional external demand matrix used in LCA studies; nonetheless, it optimizes the technosphere in terms of life cycle environmental impacts. The logic of this method is that multiple products/services with different functions can be seen as a product/service system that is serving the total demand for those functions. The method encourages the alternative scenario in which the product/service system can provide the total functional demand (i.e., the ‘combined functional unit’) relevant to those products/services with the minimum total environmental impact. For example, if ‘end products/services’ 1 and 2 are linked to the product(s)/service(s) affected by the alternative scenario, the demand matrix will be as in Eq. 4.13 and Eq. 4.14.

$$y_{old} = \begin{bmatrix} T_{1,old} \\ T_{2,old} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{matrix} \left.\vphantom{\begin{matrix} T \\ T \end{matrix}}\right\} \text{End products/ services} \\ \\ \\ \\ \\ \\ \end{matrix} \qquad \text{(Eq. 4.13)}$$

$$y_{new} = \begin{bmatrix} (F_{1,old} * t_{1,old}) * T_{1,old}/(F_{1,new} * t_{1,new}) \\ (F_{2,old} * t_{2,old}) * T_{2,old}/(F_{2,new} * t_{2,new}) \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{matrix} \left.\vphantom{\begin{matrix} T \\ T \end{matrix}}\right\} \text{End products/ services} \\ \\ \\ \\ \\ \\ \end{matrix} \qquad \text{(Eq. 4.14)}$$

In Eq. 4.13 and Eq. 4.14, *T* is the total yearly production amount of the end product/service, and subscripts ‘old’ and ‘new’ mean the baseline situation and the alternatives situation, respectively.

Once the LCI has been established with the help of Eq. 4.12, Eq. 4.13 and Eq. 4.14, this inventory can be used in the proposed environmental impact assessment model.

5. Model Application Results and Discussions

5.1. Environmental impact assessment model application results

Section 4.1 was used to guide the application of the developed environmental impact assessment model to four company cases (fabric bleacher, metal sheet priming, PU foam production, and floor coating) of different industrial branches. Section 4.1.6 and Fig. 4.3 provide explanation of the application of the ‘steps’.

5.1.1.Fabric bleacher case

Initial assessment: Identification of hazardous substances at the company level

Bleacher is one of the products that the company produces among other products such as washing powder. The company input-output data can be seen in Fig. 5.1 as the result of MFA. Company targeted sodium perborate (tetrahydrate) because of the CMR (Reprotoxic 1B) properties of the substance.

Identification of the alternatives

An alternative within an acceptable cost range for the company was found by using company experts. In terms of performance, the company also reported the efficiency of the bleacher per mass to be the same for both the baseline and the alternative situation.

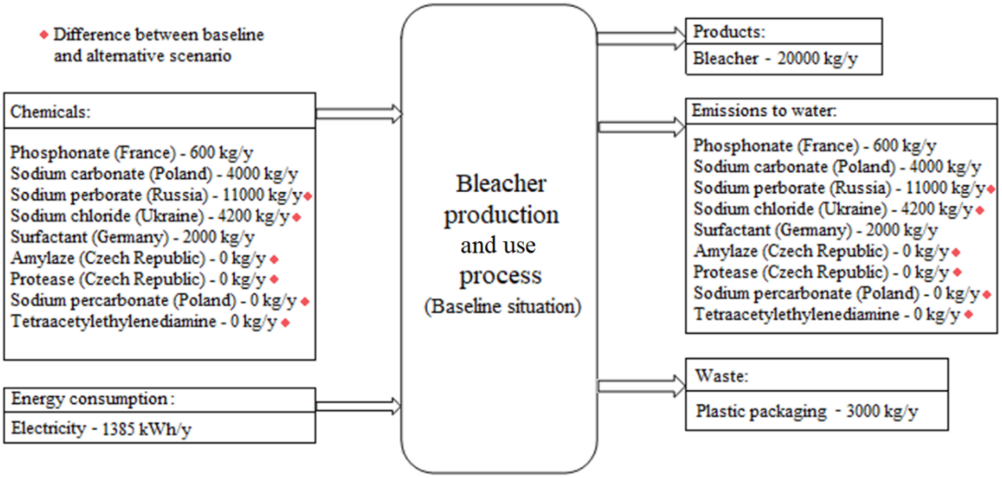

Fig. 5.1. Input-output data for baseline fabric bleacher production case

Environmental impact assessment

Step 1 and Step 2: The goal is defined as: “To compare the life cycle impacts of the substitution of sodium perborate and identify the major contributing processes.” The functional unit is defined as: “To bleach 12 full generic washing machines of clothing” (86.5 g per wash).

Step 3: As the company is an end-producer for this particular product, the boundaries of the system to be examined are defined as the fabric bleacher production process (including the supply chain) and the use phase. As it is known that the efficiencies of the products are the same both for the baseline and the alternative situation, although the company is an end-producer, the transport of the end-product, as well as the electricity and water consumption in the use phase can be excluded (now or in Step 10).

Step 4 and Step 6: as shown in Fig. 5.1 and Fig. 5.2.

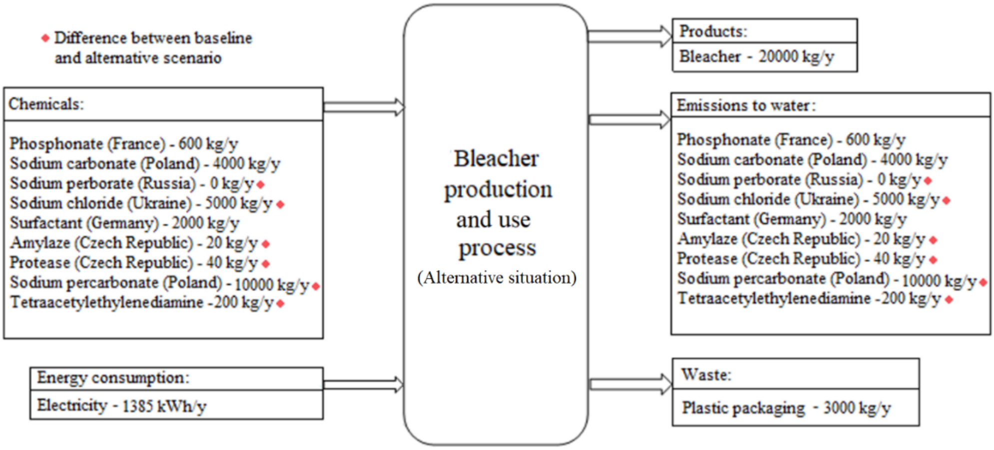

Fig. 5.2. Input-output data for alternative fabric bleacher production case

Step 5 and Step 7: The transport distance and the amount of the major input-products (sodium perborate and sodium percarbonate) for the baseline and the alternative situation were assumed to be the same, hence the transport of the input products is excluded.

Step 8 and Step 9: Step 8 was not required. In Step 9, for both the baseline and the alternative situation, the amount of the product necessary for washing 12 full generic washing machines of clothes is 1 kg.

Step 10: The common items were excluded from the company input-output data as shown in Fig. 5.1 and Fig. 5.2 (unmarked items in the figures).

Step 11, Step 12 and Step 13: In Step 11, the data was entered into SimaPro. In Step 12, sodium metaborate (a reprotoxic decomposition product of sodium perborate) could not be found in the ReCiPe method database, and the characterization factors could not be derived by using USEtox due to the lack of the octanol-water partition coefficient value for this chemical. The results obtained in Step 13 had values as indicated in Table 5.1.

Table 5.1. Results of the LCA part of the thesis model for fabric bleacher case

Damage category	Unit	Bleacher Liilia Alternative	Bleacher Liilia Baseline
Human Health	DALY	3.79E-5	1.36E-5
Ecosystems	species.yr	4.71E-8	2.13E-8
Resources	$	6.74E-2	5.73E-2

It should be noted that sodium perborate goes under a reaction when in contact with water producing hydrogen peroxide and sodium metaborate, and, although sodium metaborate is known to be reprotoxic (Scientific Committee on Consumer Safety [SCCS], 2010) and is being released in relatively high amounts in the current case, characterization factors for this chemical do not exist in the ReCiPe methodology. Also, it was not possible to calculate characterization factors by using USEtox. Hence, unfortunately, the results of the simplified LCA exclude the reprotoxic effects of this particular emission.

Step 14 and Step 15: Representative life cycle processes of the fabric bleacher baseline and alternative cases listed in Table 5.2 and Table 5.3, respectively.

Table 5.2. Representative life cycle processes of fabric bleacher classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the baseline situation

Representative life cycle processes and their output amounts						
0.55 kg Sodium perborate (2)	0.21 kg Sodium chloride (2)	0.01 kg Sulphur reduction of diesel (2)	2.90E-3 kg Quicklime milling (2)	2.90E-3 kg Quicklime production (2)	2.70E-3 kg Soda (2)	6.90E-2 tkm Train (2)
0.29 tkm transport, ship (1)	8.6E-3 tkm Light vehicle (2)	0.28 tkm Lorry (7)	0.01 MJ Heat, heavy fuel oil (1)	0.03 MJ Heat, wood (4)	0.02 MJ Heat, coal/lignite (5)	5.5E-3 MJ Electricity production, hard coal (2)
0.06 MJ Hard coal[1] (1)	1.00 MJ Diesel production, petroleum refinery[2] (3)	0.01 MJ Heavy fuel oil[3]	0.03 MJ Coal/lignite/ hard coal[3]			

104 nodes, 40 non-market processes (excluding voltage transformation and road construction (infrastructure))

[1] Hard coal lower heating value: 26.3 MJ/kg (JRC, 2017);

[2] Diesel heating value: 42.96 MJ/kg (JRC, 2017);

[3] Upstream fuel operation for some part of electricity derived (90% plant efficiency assumed)

Table 5.3. Representative life cycle processes of fabric bleacher classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the alternative scenario

Representative life cycle processes and their output amounts						
3.00E-3 kg Enzyme, alpha amylase (1)	0.50 kg Sodium percarbonate (2)	0.26 kg Sodium chloride (2)	0.01 kg EDTA chemical (2)	7.23E-3 tkm Light vehicle (1)	0.26 tkm Lorry (5)	0.03 MJ Heat, coal/lignite (5)
2.90E-3 kg Wood chips, dry (1)	9.40E-3 kg Soda ash (2)	3.20E-3 kg Hydrogen cyanide (2)	1.70E-3 kg Ethylene diamine (2)	5.40E-3 kg Sodium cyanide (2)	0.04 MJ Heat, from wood (3)	3.70E-3 MJ Electricity production, hard coal (1)
0.32 tkm Transport, ship (1)	2.40E-3 kg Quicklime milling (1)	2.40E-3 kg Quicklime (1)	0.01 kg Sulfur reduction of diesel (2)	1.90E-3 kg Ethylene dichloride (1)	0.09 MJ Hard coal[1] (1)	0.48 MJ Diesel, petroleum refinery[2] (2)
0.04 MJ Coal/lignite/hard coal[3]						

104 nodes, 40 non-market processes (excluding voltage transformation and road construction (infrastructure))

[1] Hard coal lower heating value: 26.3 MJ/kg (JRC, 2017);

[2] Diesel heating value: 42.96 MJ/kg (JRC, 2017);

[3] Upstream fuel operation for some part of electricity derived (90% plant efficiency assumed)

Step 16: The DALYs for each NACE Rev. 2 activity can be seen in Table 5.4 (Annex I provides details regarding derivation).

Table 5.4. Work environment DALY per total production amount and color code for each economic sector (color code only for Section 5)

WE_DALY per unit output	**NACE Rev. 2 classification**
2.47222172E-8 y/kg	A01 – Crop and animal production, hunting and related service activities
2.1051054E-10 y/MJ	B05 – Mining of coal and lignite
2.3051688E-11 y/MJ	B06 – Extraction of crude petroleum and natural gas
1.3328933E-11 y/MJ	C19 – Manufacture of coke and refined petroleum products
4.23942927E-9 y/kg	C20 – Manufacture of chemicals and chemical products
7.3223715E-11 y/MJ	D35 – Electricity, gas, steam and air conditioning supply
1.0458336E-8 y/t*km	H49 – Land transport and transport via pipelines

Step 17: Life cycle accident impacts of fabric bleacher case are shown in Table 5.5.

Table 5.5. WE-CFs method results for fabric bleacher case in DALY units

NACE Rev. 2 activity	Fabric bleacher Baseline situation (years)	Fabric bleacher Alternative situation (years)
C20	3.31E-9	3.43E-9
H49	6.76E-9	6.16E-9
D35	4.74E-12	5.72E-12
C19	1.35E-11	6.41E-12
B05	1.90E-11	2.68E-11
A01	-	7.19E-11
Total:	**1.01E-8**	**9.69E-9**

Step 18, Step 19 and Step 20: Cancer/non-cancer scores of intermediate chemicals concerning fabric bleacher case can be seen in Table 5.6 and Table 5.7 (see Annex II). The chemicals in used did not have any toxicity values.

Step 21: Detailed results of the Modified LCIT method for the fabric bleacher case are presented in Table 5.8 and Table 5.9 (see Annex II).

Step 22 and Step 23: Final results after normalization and weighting are given in Table 5.10.

Table 5.10. Total normalized and weighted results for fabric bleacher case, excluding modified LCIT 'water emissions', RA and usage/emission amounts

	Simplified LCA			**1.90E-3*Modified LCIT 'air emissions'**			
Situations	**Human Health**	**Ecosystems**	**Resources**	**Human Health**	**Ecosystems**	**WE-CFs**	**Total[1,2]**
Unit	**DALY**	**species.yr**	**$**	**DALY**	**species.yr**	**DALY**	**-**
Baseline	1.36E-5	2.13E-8	0.06	0	0	1.01E-8	**2.00E-1**
Alternative	3.79E-5	4.71E-8	0.07	1.52E-10	2.83E-12	9.69E-9	**4.81E-1**

[1] Except modified LCIT 'water emissions';

[2] LCIT method results included

For RA, PROC 5 and PROC 8b were found to be appropriate. ERC 8b was adopted. Due to the disassociation of sodium perborate in water, boron and hydrogen peroxide toxicities were used with the precautionary principle for the environmental risk derivation as suggested in the registration dossier of sodium perborate by ECHA. RA results for the bleacher case are given in Table 5.11.

Table 5.11. Risk assessment results for bleacher case

	Workers RCR (above 1)	**Consumers RCR (above 1)**	**Environment RCRs (above 1)**
Baseline situation	No	Yes	No
Alternative situation	No	No (Sodium percarbonate data missing)	No

Usage/emission amounts method results for the bleacher case are outlined in Table 5.12 and Table 5.13.

Table 5.12. Usage/emissions amounts results for baseline situation of bleacher case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	0	0.55	0
	Endocrine disruption	0	0	0
	Highly flammable/explosive/reactive	N/A	N/A	0.55
	Carcinogenic/mutagenic	0	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	0	0.55	0
	Endocrine disruption	0	0	0
	PBT and vPvB	N/A	N/A	0
	Carcinogenic/mutagenic	0	N/A	N/A

Table 5.13. Usage/emissions amounts results for alternative situation of bleacher case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	Highly flammable/explosive/reactive	N/A	N/A	0.50
	Carcinogenic/mutagenic	0	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	PBT and vPvB	N/A	N/A	0
	Carcinogenic/mutagenic	0	N/A	N/A

Evaluation of the results and implementation

The company decided to implement the alternative situation due to the reduction in reprotoxicity and reduction of risk to consumers. However, an increase in life cycle impacts raised questions regarding the success of the substitution. If normalization factors for usage/emission amounts (as derived in Section 2.6) had been used, then human health impact results of usage/emission amounts (excluding physical hazards) (8.00E-7 DALY) would be negligible compared to the life cycle impact results (1.36E-5 DALY) as presented in Table 5.10. The normalization of human health impact results and ecosystem impact results (by using the normalization values outlined in Section 4.1.6) indicates that the ecosystem impacts are in the range of a quarter to one fifth of the overall human health impacts. Hence the baseline situation would be preferable.

The contribution of the WE-CFs method to the human health scores was ignorable when compared to the results derived by the Simplified LCA method (Table 5.1 and Table 5.5 in Section 5.1.1). However, this might not always be the point for other cases, as Scanlon *et al*. (2015) showed that, for the waste treatment stage, this is not true. The same point is valid for the usage/emission method. This is considered to be due to the higher number of public population compared to the considered worker population in this specific case. The worker health results of the WE-CFs (accidents at work) method were comparable to the human health impact (due to fugitive and accidental emissions) results of the Modified LCIT method. Also, the WE-CFs method focuses more on accidents that can be linked directly to the production process, such as physical accidents, but LCA takes into account a different set of impact pathways. The major contributor to the human health impact and the ecosystem impact in the alternative scenario was the sodium percarbonate production. The exclusion of sodium metaborate emissions increased the uncertainty on the toxicity impacts, especially reprotoxicity. Chlorine emissions contributed the most to freshwater ecotoxicity, whereas beryllium emissions contributed the most to marine ecotoxicity. Major human health impact contributors for the sodium percarbonate production process are selenium, manganese and chlorine emissions into the water compartment. LCA does not consider the benefits of micronutrients that are necessary in small amounts but toxic in high amounts. Instead, it assumes a linear relationship for toxicity even at low doses. Due to these facts, the validity of the obtained human toxicity results could not be concluded. The LCA results for human toxicity could not be validated due to the lack of consideration of micronutrients and reprotoxicity in the ReCiPe methodology and the missing important data in the LCI database.

The occupational safety part of the LCIT method yielded no results due to the lack of effect factors in the USEtox database for the given chemicals as these chemicals are not considered to be highly toxic.

The Simplified LCA results showed a higher ecological impact due to the production of the chemicals EDTA and Ethylene diamine. Overall, the life cycle environmental impact increased by 140% due to substitution.

The use of CAS numbers was found to be more appropriate than the EC numbers due to the inability of the EC numbers to distinguish between hydration (e.g., monohydrate, tetrahydrate) forms of chemicals.

5.1.2.Metal sheet priming case

Initial assessment: Identification of hazardous substances at the company level

The main focus of the metal sheet priming company is cleaning, priming, and cutting steel sheets and profiles which are mostly intended for ship building.

A detailed description of the process is as follows:

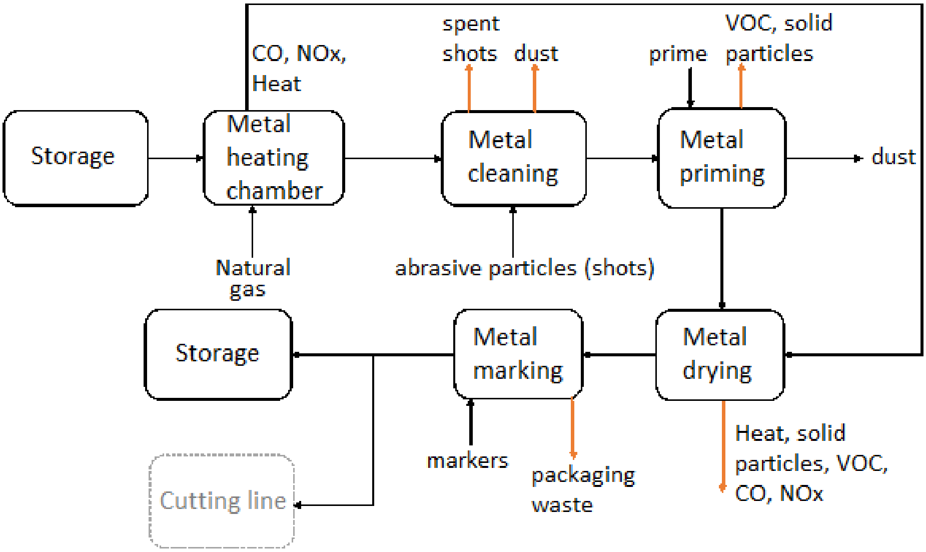

Fig. 5.3. Flowchart of technological line for cleaning and priming

The cleaned metal goes to priming, where dyes are sprayed onto the metal surface. The dye mist which forms during the spraying process is drawn off to the rotary brush chamber where air is cleaned to the required quality and emitted into the atmosphere. The metal surface gets covered with 15–50 µm two component zinc ethyl silicate inter-operational primer which is solvent-based and intended for automatic sprayers.

After the priming, metal is directed to drying in the drying chamber. The excess heat from the heating chamber is used there. Volatile organic compounds (VOCs) that are present in dyes are emitted into the air both during the processes of metal priming and drying.

VOCs and 2-methoxypropanol (a reprotoxic chemical) were reported as reasons for substitution.

The input-output data was reported by the company as in Fig. 5.4.

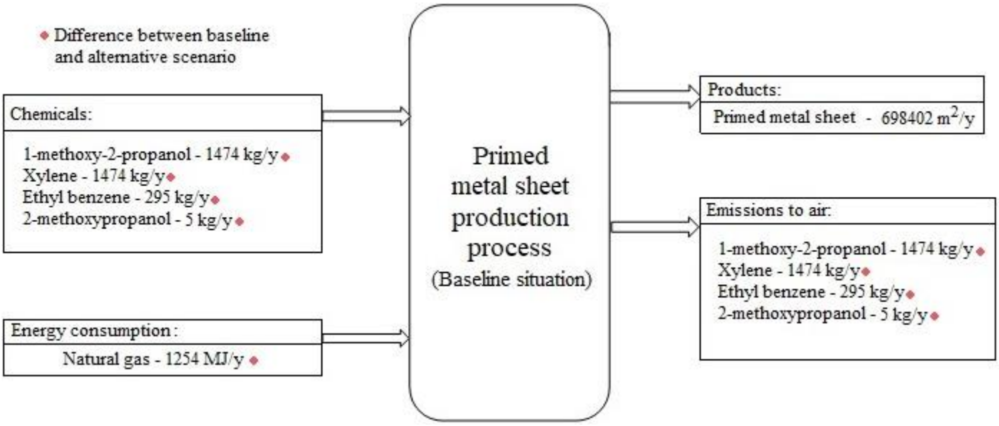

Fig. 5.4. Input-output data for baseline situation (‘Thinner 1’). Only the inventory difference between baseline and alternative scenario is shown

A detailed inventory of the used chemicals is presented in Table 5.14 (refer to Annex II).

Identification of the alternatives

The company identified two possible alternatives by using company contacts: a water-based and a solvent-based shop primer. The water based paint was found to be unacceptable from the technical point of view. The company preferred the solvent-based alternative due to its economic and technical suitability.

Environmental impact assessment

Step 1 and Step 2: The goal was defined as: “To compare the life cycle impacts of the substitution of ‘Thinner 1’ with ‘Thinner 2’ and identify major contributing processes.” The functional unit was defined as: “Production of 1 m^2 primed metal sheet.”

Step 3: As the manufactured product was not changed in any aspect after the substitution, the scope of the assessments will exclude the use phase of the product.

Step 4 and Step 6: We refer to Fig. 5.4 and Fig. 5.5.

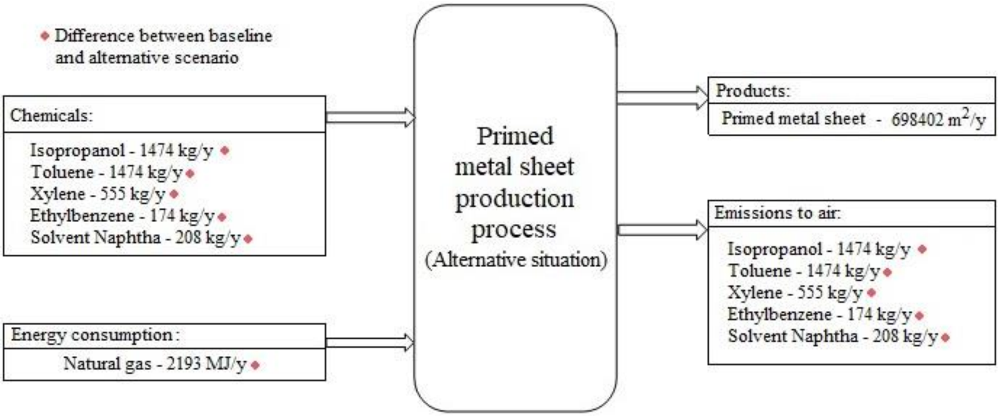

Fig. 5.5. Input-output data for alternative situation (‘Thinner 2’). Only the inventory difference between baseline and alternative scenario are shown

Step 5 and Step 7: Transportation of the thinner products was assumed to be over the distance of 1,700 km (road transportation from Germany to Lithuania).

Propylene glycol methyl ether (1-methoxy-2-propanol or propylene glycol monomethyl ether) could not be found in the LCA database; hence a close derivative, i.e., dipropylene glycol monomethyl ether (often used as a less volatile alternative to propylene glycol methyl ether), was assumed to be used instead.

Step 8 and Step 9: Step 8 was not required. In Step 9, the company’s input-outputs were normalized to the production of 1 m^2 of primed metal sheet.

Step 10: The uncommon items can be seen as marked in Fig. 5.4 and Fig. 5.5.

Step 11 and Step 12: The data was entered into the LCA software. Step 12 was not needed.

Step 13: The results were obtained as in Table 5.15.

Table 5.15. Results of the LCA part of the methodology for metal sheet priming case

Damage category	Unit	Metal sheet priming Alternative	Metal sheet priming Baseline
Human Health	DALY	4.78E-8	1.28E-7
Ecosystems	species.yr	1.89E-10	2.95E-10
Resources	$	1.40E-3	1.40E-3

Step 14 and Step 15: Representative life cycle processes of the metal sheet priming baseline and alternative cases are listed in Table 5.16 and Table 5.17, respectively.

Table 5.16. Representative life cycle processes of metal sheet priming case classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the baseline situation

Representative life cycle processes and their output amounts						
2.10E-3 kg Dipropylene Glycol Monomethyl Ether (2)	2.10E-3 kg Xylene (2)	4.20E-4 kg Ethylbenzene (2)	4.00E-3 kg Sodium Chloride (2)	1.70E-3 kg Propylene oxide (2)	1.30E-3 kg Propylene (2)	2.30E-3 kg Chlorine (2)
3.20E-4 kg Benzene (2)	4.80E-4 kg Methanol (1)	7.70E-5 kg Ethylene (1)	4.00E-4 kg Sulfur reduction of diesel (1)	0.02 MJ Diesel, Petroleum refinery[1] (1)	0.01 MJ Hard coal mining[2] (1)	9.00E-3 tkm Lorry transport (2)
8.40E-3 MJ heat, natural gas (5)	1.40E-4 MJ Heat, hard coal (1)	5.40E-3 MJ electricity (12)	3.70E-3 MJ Hard coal/lignite[3]	9.30E-3 MJ Natural gas[3]	1.60E-4 MJ Hard coal[3]	

122 nodes, 43 non-market processes in total (excluding voltage transformation because already included in the ‘electricity supply’ accidents per output of electricity)

[1] Diesel heating value: 42.96 MJ/kg (JRC, 2017);

[2] Hard coal lower heating value: 26.3 MJ/kg (JRC, 2017);

[3] Upstream fuel operation for some part of the electricity derived (90% plant efficiency assumed)

Table 5.17. Representative life cycle processes of metal sheet priming case classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the alternative situation

Representative life cycle processes and their output amounts						
2.11E-3 kg Isopropanol (2)	2.11E-3 kg Toluene (2)	8.00E-4 kg Xylene (2)	2.50E-4 kg Ethylbenzene (2)	9.10E-11 kg Zinc (1)	9.50E-3 tkm Lorry transport (1)	4.63E-4 kg Diesel, low sulfur (1)
-1.60E-3 MJ electricity (7)	4.81E-3 MJ heat, natural gas (4)	1.56E-3 kg Propylene (2)	3.69E-3 MJ Steam[1] (2)	1.89E-4 kg Benzene (2)	2.58E-4 MJ heat, wood chips (2)	6.73E-4 MJ heat, hard coal/lignite (4)
-3.80E-6 kg Clinker (2)	1.00E-2 MJ Diesel[2], Petroleum refinery (1)	-7.96E-5 kg Cement (2)	6.94E-4 MJ Heat, heavy fuel oil (1)	-2.52E-3 kg Treatment of digester sludge (1)	-3.08E-5 m^3 Biogas, anaerobic digestion of manure (1)	1.47E-2 MJ Naphtha[3], Petroleum refinery (1)
-1.32E-3 MJ Hard coal/lignite[4]	-2.68E-4 MJ Oil[4]	5.35E-3 MJ Natural gas[4]	7.5E-4 MJ Hard coal/lignite[4]	7.7E-4 MJ Heavy fuel oil[4]		

96 nodes, 43 non-market processes in total

[1] Steam: 2.26 MJ/kg latent heat;

[2] Diesel heating value: 42.96 MJ/kg (JRC, 2017);

[3] Naphtha heating value: 44 MJ/kg (JRC, 2017);

[4] Upstream fuel operation for some part of the electricity derived (90% plant efficiency assumed)

Step 16: Refer to Table 5.4 in Section 5.1.1.

Step 17: Life cycle accident impacts of the metal sheet priming case are shown in Table 5.18.

Table 5.18. WE-CFS method results for metal sheet priming case in DALY units

NACE Rev. 2 activity	**Metal sheet priming Baseline situation (years)**	**Metal sheet priming Alternative situation (years)**
C20	6.48E-11	2.06E-11
H49	9.38E-11	9.89E-11
D35	1.02E-12	6.24E-13
C19	2.30E-13	4.72E-13
B05	3.98E-12	-1.19E-13
B06	2.14E-13	1.17E-13
Total:	**1.68E-10**	**1.21E-10**

Step 18, Step 19 and Step 20: The cancer/non-cancer scores of intermediate chemicals concerning the metal sheet priming case are listed in Table 5.19 and Table 5.20 (see Annex II). For the baseline situation, a cancer score of 9.29E-5 and a non-cancer score of 8.35E-4 were obtained. In the alternative situation, a cancer score of 1.29E-5 and a non-cancer score of 1.97E-5 were obtained.

Step 21: Detailed results of the Modified LCIT method for metal sheet priming case are outlined in Table 5.21 and Table 5.22 (refer to Annex II).

Step 22: Results after normalization and weighting are given in Table 5.23.

Table 5.23. Total normalized and weighted results for metal sheet priming case, excluding modified LCIT 'water emissions', RA and usage/emission amounts

	Simplified LCA			**1.90E-3*Modified LCIT 'air emissions'**			
Situations	**Human Health**	**Ecosystems**	**Resources**	**Human Health**	**Ecosystems**	**WE-CFs**	**Total^{1,2}**
Unit	**DALY**	**species.yr**	**$**	**DALY**	**species.yr**	**DALY**	**-**
Baseline	1.28E-7	2.95E-10	0.00135	4.26E-10	1.94E-13	1.68E-10	**2.59E-3**
Alternative	4.78E-8	1.89E-10	0.00136	8.44E-13	2.34E-17	1.21E-10	**1.62E-3**

[1] Except for modified LCIT 'water emissions';

[2] LCIT method results included

For RA, PROC 7 and ERC 4 were adopted. The RA results for metal sheet production case are given in Table 5.24.

Table 5.24. Risk assessment results for metal sheet priming case

	Workers RCR (above 1)	**Consumers RCR (above 1)**	**Environment RCRs (above 1)**
Baseline situation	No	N/A	Yes (except man via environment)
Alternative situation	No	N/A	Yes (except man via environment)

The usage/emission amounts method results for the metal sheet production case can be seen in Table 5.25 and Table 5.26.

Table 5.25. Usage/emission amounts results for baseline situation of metal sheet priming case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	0	7.16E-6	0
	Endocrine disruption	0	0	0
	Highly flammable/explosive/reactive	N/A	N/A	8.76E-3
	Carcinogenic/mutagenic	4.80E-4	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	PBT and vPvB	N/A	N/A	0
	Carcinogenic/mutagenic	0	N/A	N/A

Table 5.26. Usage/emission amounts results for alternative situation of metal sheet priming case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	2.11E-3	0	0
	Endocrine disruption	0	0	0
	Highly flammable/explosive/reactive	N/A	N/A	7.01E-3
	Carcinogenic/mutagenic	0	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	2.11E-3	0	0
	Endocrine disruption	0	0	0
	PBT and vPvB	N/A	N/A	0
	Carcinogenic/mutagenic	0	N/A	N/A

Evaluation of the results and implementation

The identification of alternatives was a complicated and time resource-demanding process. The company tested water-based alternatives which were found not to work.

The ecosystem impacts were in the range between one third to a half of human health impacts. The improvement in all impacts (except for an increase in the usage/emission of substances with suspected reprotoxicity) indicated the success of substitution. The usage/emissions amounts method result (3.07E-9 DALY) for impacts (if normalization was applied as described in Section 2.6) of the suspected reprotoxics for an alternative situation does not change this conclusion. Also, this increase in the use of a suspected reprotoxic substance (toluene) was tolerated due to the assurance from ECHA on the toluene's safety in industrial setups. An alternative situation was preferable almost in all aspects concerning environmental impacts (with a 37% reduction in the life cycle environmental impacts); only an increase in the use and emission of chemicals with suspected reprotoxicity and the local risk to some environmental compartments raised concerns about the success of the substitution. This increase in reprotoxicity was due to the use of toluene as a component of the substitute.

5.1.3. PU foam production case

Initial assessment: Identification of hazardous substances at the company level

The researched polyurethane (PU) foam production company is a supplier of one component – polyurethane foams – globally. The production process includes raw materials mixing and packing into pressurized containers. Additionally, the company is packing silicones, acrylic and bitumen materials into retail packaging.

The production process can be seen in Fig. 5.6:

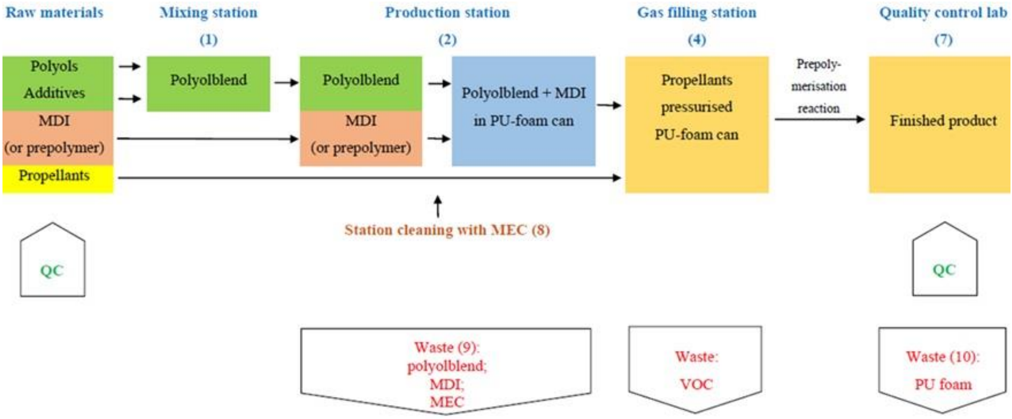

Fig. 5.6. Production process of polyurethane foam (pressured can product) in the company. Here, QC represents ‘Quality Control’

The input-output data was reported by the company as in Fig. 5.7.

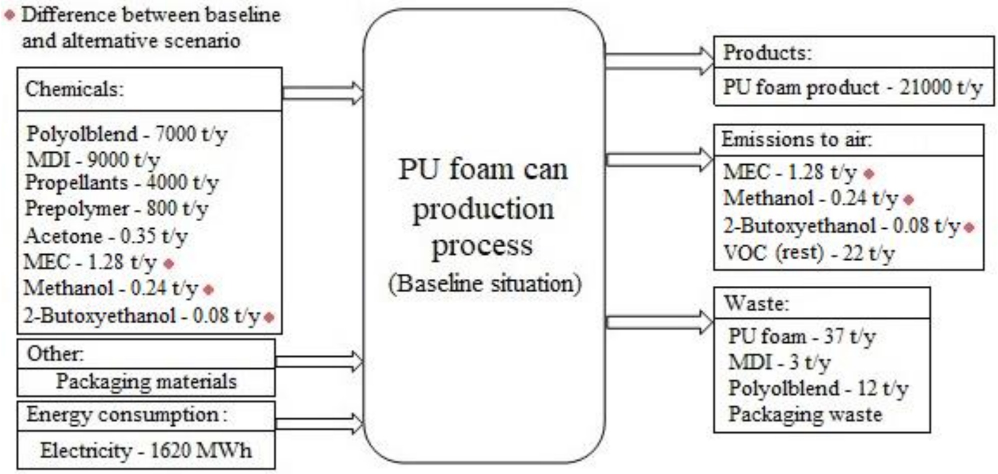

Fig. 5.7. Input-output data for the baseline situation in the production of canned PU foam product

The production of one component – polyurethane foam – is the process of concern. In some special products, the production uses prepolymer as a raw material which is highly viscous and sticky. Currently, methylene chloride (MEC), also known as dichloromethane, is used for cleaning the mechanical components exposed to prepolymer. MEC is a suspected carcinogen according to ECHA. Therefore, the company was targeting to substitute it with a cleaning agent which is not classified as hazardous.

Identification of the alternatives

According to a research by TURI of UMASS Lowell (Morose *et al.*, 2017), a safer alternative to MEC with comparable performance was identified by using the GreenScreen method. The alternative contains methyl acetate, dimethyl sulfoxide (DMSO) and thiophene. As the amount of the MEC cleaner for the baseline situation was reported as 1.6 t/y, it was possible to derive the possible components of this product as indicated in Fig. 5.8 by using the data on MEC-based cleaners as reported by the same study (Morose *et al.*, 2017) while ignoring the components that are less than 5% by weight. However, for the alternative case, the quantitative information about the composition of the cleaner was kept secret from the public, and it was not possible to find any quantitative data on this issue. Due to the lack of information, assumptions had to be made as follows: the composition of the DMSO-based cleaner is 60% methyl acetate, 30% DMSO, and 10% thiophene.

Environmental impact assessment

Step 1 and Step 2: The goal is defined as: “To compare the life cycle impacts of the substitution of the MEC-based cleaner with a DMSO-based cleaner and identify the major contributing processes.” The functional unit is defined as: “The production of 1 kg canned PU foam.”

Step 3: As the manufactured product was not changed in any aspect after the substitution, the scope of the assessments will exclude the use phase of the product.

Step 4 and Step 6: Refer to Fig. 5.7 and Fig. 5.8.

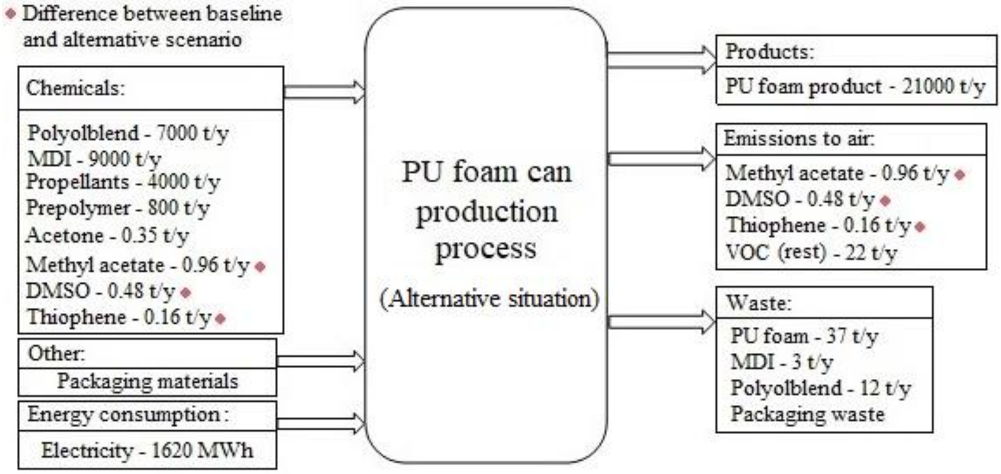

Fig. 5.8. Input-output data for the assumed alternative situation in the production of canned PU foam product

Step 5 and Step 7: For the baseline situation, 2-butoxyethanol was missing from the inputs from technosphere in the LCA database. Hence, the production process of this chemical and its transportation were excluded from the LCA inventory, and instead its parent chemicals 1-butanol (63% bw) and ethylene oxide (37% bw) were used (Harris *et al*., 1998).

Similarly, for the alternative scenario, Thiophene was missing from the inputs from technosphere in the LCA database. Hence, the production process of this chemical and its transportation were excluded from the LCA inventory, and instead its parent chemicals 1-butanol (49% bw) and carbon disulfide (51% bw) were used (Swanston, 2006).

Step 8 and Step 9: Step 8 was not required. In Step 9, the company’s input-outputs were normalized to the production of 1 kg canned PU foam product.

Step 10: The uncommon items can be seen as marked in Fig. 5.7 and Fig. 5.8.

Step 11and Step 12: The data was entered into the LCA software. Step 12 was not required.

Step 13: The obtained results were as shown in Table 5.27.

Table 5.27. Results of the LCA part of the methodology for PU foam production case

Damage category	**Unit**	**PU foam Alternative**	**PU foam Baseline**
Human Health	DALY	8.39E-10	2.22E-9
Ecosystems	species.yr	2.51E-12	6.64E-12
Resources	$	1.49E-5	9.44E-6

Step 14 and Step 15: Representative life cycle processes of the PU foam production baseline and alternative cases are listed in Table 5.28 and Table 5.29, respectively.

Table 5.28. Representative life cycle processes of PU foam production case classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the baseline situation

Representative life cycle processes and their output amounts						
6.10E-5 kg Dichloromethane (2)	1.14E-5 kg Methanol (1)	1.43E-6 kg Ethylene oxide (2)	2.38E-6 kg 1-butanol (2)	2.44E-6 kg Cement (2)	4.41E-7 kg Oxygen (1)	-1.79E-6 kg Clinker[1] (1)
1.18E-6 kg Ethylene (Ethene) (2)	6.49E-7 kg Carbon monoxide (1)	1.95E-6 kg Clinker (1)	1.42E-6 kg Propylene (Propene) (2)	1.65E-6 kg Average incineration residue treatment (1)	8.55E-12 kg Zinc (1)	2.90E-7 kg Wood chips, dried (1)
1.32E-5 MJ Heat, coal/lignite (4)	2.64E-5 MJ Heat from natural gas (4)	-2.27E-5 MJ Electricity[1] (10)	1.49E-6 MJ Heat, wood (1)	4.41E-5 t*km Transport, ship (1)	1.55E-6 tkm Lorry (2)	6.79E-5 MJ Natural gas[2] (1)
-2.25E-7 m^3 Biogas, manure anaerobic digestion (1)	-1.84E-5 kg digester sludge treatment (1)	-1.70E-5 MJ Hard coal/lignite[3]	-4.50E-6 MJ Natural gas[3]	-2.80E-6 MJ Oil[3]	1.50E-5 MJ Coal/lignite[3]	2.90E-5 MJ Natural gas[3]

104 nodes, 45 non-market processes in total

[1] Negative values indicate the deduction of the process from the technosphere (due to the substitution/system expansion method intended to eliminate the co-products in the joint processes as suggested by ISO 14044);

[2] Natural gas standard heating value: 39 MJ/m^3 (IGU, 2012);

[3] Upstream fuel operation for some part of the produced electricity (90% plant efficiency assumed)

Table 5.29. Representative life cycle processes of PU foam production case classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the alternative situation

Representative life cycle processes and their output amounts						
1.02E-6 kg Oxygen (1)	2.63E-6 kg 1-butanol (2)	4.57E-5 kg Methyl acetate/ Organic solvent (1)	2.33E-5 kg Methanol (1)	8.18E-6 kg Propylene (2)	5.01E-6 kg Cumene (2)	2.04E-6 kg Cyclohexanol (1)
3.05E-6 kg Dichloromethane (2)	2.04E-6 kg Ethylbenzene (1)	2.71E-6 kg Ethylene Glycol (1)	2.01E-6 kg Isopropanol (1)	2.10E-6 kg Methyl ethyl ketone (1)	3.05E-6 kg Styrene (2)	2.61E-6 kg Tetrachloroethylene (1)
8.95E-6 kg Benzene (2)	2.286E-5 kg Dimethyl sulfoxide (2)	2.58E-6 kg Xylene (1)	2.04E-6 kg Nitrobenzene (1)	2.04E-6 kg Acetone (1)	1.87E-6 kg Carbon monoxide (1)	1.45E-6 kg Ethylene oxide (1)
9.78E-7 kg Phenol (1)	7.85E-6 MJ Heat, coal/lignite (2)	2.27E-4 MJ Heat, natural gas (4)	-3.67E-5 MJ Electricity[1] (4)	1.21E-6 kg Hazardous waste incineration (1)	2.69E-6 kg Toluene (1)	-6.84E-7 m^3 Biogas, anaerobic digestion[1] (1)
-5.59E-5 kg Digester sludge treatment[1] (1)	-3.00E-5 MJ Hard coal[2]	-8.00E-6 MJ Oil[2]	9.00E-6 MJ Coal/lignite[2]	2.53E-4 MJ Natural gas[2]		

102 nodes, 43 non-market processes

[1] Negative values indicate the deduction of the process from the technosphere (due to the substitution/system expansion method intended to eliminate the co-products in the joint processes as suggested by ISO 14044);

[2] Upstream fuel operation for some part of the produced electricity (90% plant efficiency assumed);

Step 16: Refer to Table 5.4 in Section 5.1.1.

Step 17: Life cycle accident impacts of the PU foam production case can be seen in Table 5.30.

Table 5.30. WE-CFs method results for PU foam production case in DALY units

NACE Rev. 2 activity	**PU foam production Baseline situation (years)**	**PU foam production Alternative situation (years)**
C20	2.79E-13	4.079E-13
H49	4.77E-13	-
B06	2.06E-15	5.64E-15
D35	1.35E-15	1.45E-14
A01	7.17E-15	-
B05	-4.21E-16	-4.42E-15
Total:	**7.68E-13**	**4.24E-13**

Step 18, Step 19 and Step 20: Cancer/non-cancer scores of intermediate chemicals concerning the PU foam production case can be seen in Table 5.31 and Table 5.32 (refer to Annex II). For the baseline situation, a cancer score of 5.39E-7 and a non-cancer score of 2.67E-6 were obtained. In the alternative situation, a cancer score of 1.01E-6 and a non-cancer score of 1.41E-6 were obtained.

Step 21: Detailed results of the Modified LCIT method for PU foam production case are outlined in Table 5.33 and Table 5.34 (refer to Annex II).

Step 22 and Step 23: Results after normalization and weighting are presented in Table 5.35.

Table 5.35. Total normalized and weighted results for PU foam production case, excluding modified LCIT 'water emissions', RA and usage/emission amounts

	Simplified LCA			**1.90E-3*Modified LCIT 'air emissions'**			
Situations	**Human Health**	**Ecosystems**	**Resources**	**Human Health**	**Ecosystems**	**WE-CFs**	**Total^{1,2}**
Unit	**DALY**	**species.yr**	**$**	**DALY**	**species.yr**	**DALY**	**-**
Baseline	2.22E-9	6.64E-12	9.44E-6	2.15E-12	5.85E-15	7.68E-13	**3.75E-5**
Alternative	8.39E-10	2.51E-12	1.49E-5	1.47E-12	3.12E-16	4.24E-13	**2.17E-5**

[1] Except for modified LCIT 'water emissions';

[2] LCIT method results included

For RA, PROC 10 and ERC 4 were adopted. The RA results for the PU foam production case are listed in Table 5.36.

Table 5.36. Risk assessment results for PU foam production case

	Workers RCR (above 1)	**Consumers RCR (above 1)**	**Environment RCRs (above 1)**
Baseline situation	No	N/A	All, human via environment unknown
Alternative situation	No (Thiophene toxicities missing)	N/A	All, human via environment unknown (Thiophene toxicities missing)

The usage/emission amounts method results for the PU foam production case are listed in Table 5.37 and Table 5.38.

Table 5.37. Usage/emission amounts results for baseline situation of PU foam production case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	Highly flammable/explosive/reactive	N/A	N/A	1.82E-5
	Carcinogenic/mutagenic	7.24E-5	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	PBT and vPvB	N/A	N/A	0
	Carcinogenic/mutagenic	1.14E-5	N/A	N/A

Table 5.38. Usage/emission amounts results for alternative situation of PU foam production case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	5.74E-6	2.04E-6	0
	Endocrine disruption	0	0	0
	Highly flammable/explosive/reactive	N/A	N/A	1.15E-4
	Carcinogenic/mutagenic	3.20E-5	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	PBT and vPvB	N/A	N/A	0
	Carcinogenic/mutagenic	0	N/A	N/A

Evaluation of the results and implementation

The ecosystem impacts were approximately a half of the level of human health impacts. The methods thus yielded opposing results. Substitution was a success when the life cycle impacts were considered. If normalization had been applied to the usage/emission amounts method as suggested in Section 2.6, the impacts of the usage/emission amounts would be negligible to the life cycle impact results, hence this conclusion would not change.

The results indicate that the environmental impacts including the human health impacts from intended and accidental/fugitive emissions decreased in the alternative scenario, i.e., when reprotoxicity was ignored. The WE-CFs results also indicate that the upstream worker's safety regarding physical accidents was improved, although the usage/emission amounts indicate an increase in the use of highly flammable/explosive/reactive substances in the upstream. The overall life cycle environmental impacts declined by 42%. The LCIT method and the usage and emission amounts suggest that impacts of carcinogenic substances on upstream workers decreased by 56%. However, potential reprotoxicity and non-cancer toxicity impacts on workers increased according to the usage and emission amounts and the LCIT method, respectively. The risk assessment results yielded no difference except for the uncertainty in risk to workers, as the risk from Thiophene was uncertain.

5.1.4.Floor coating case

Initial assessment: Identification of hazardous substances at the company level

The company is manufacturing two-component epoxy resin systems which are used as floor coatings. Two-component epoxy resins are meant for professional use only.

The product contains about 70% of the resin (component A) and 30% of the hardener (component B) which are mixed together at the site where the flooring system is installed. The production process does not include any chemical reactions, such as synthesis or thermal processing, but only mixing certain chemicals (mixtures) according to the recipes. The VOC amounts from the production were reported to be relatively low (0.1727 kg/year). Benzyl alcohol was reported as the only ingredient that will be emitted into indoor air during the use phase (within 6 months), and all the other ingredients involve low vapor pressures, and they are incorporated into the product after curing (with a curing time within 8 to 24 hours).

In 2015, nonylphenol (reproductive toxicity, category 2) was contained in the hardener of the topmost layer in 3-layer epoxy-flooring.

The input-output data was reported by the company as in Fig. 5.9.

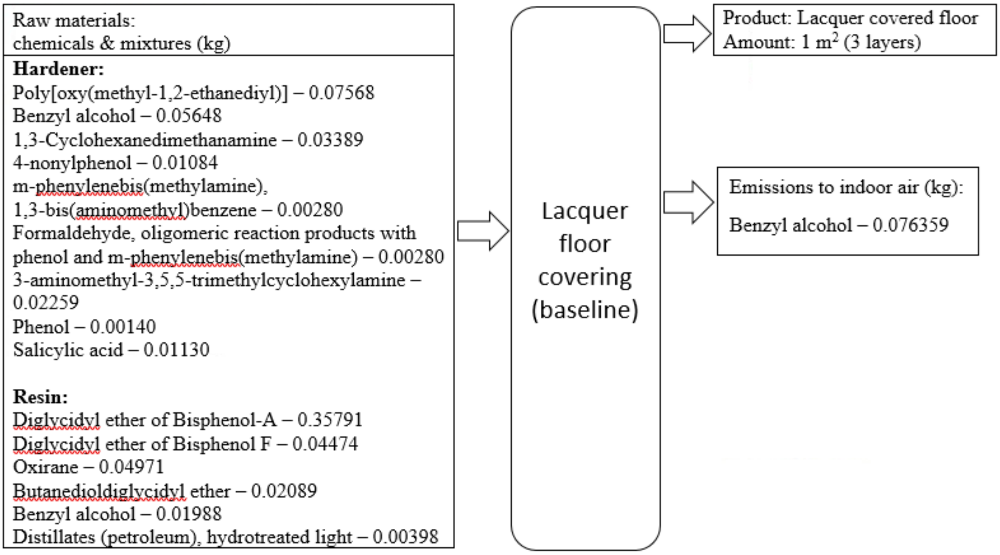

Fig. 5.9. Input-output data for the baseline situation in the production of three-layer coated floor in 2015. Only the changed components are shown

Identification of the alternatives

The company identified technically and economically suitable alternatives by company contacts.

Environmental impact assessment

Step 1 and Step 2: The goal is defined as: "To compare the life cycle impacts of the substitution of nonylphenol containing floor coating with a nonylphenol-free alternative." The functional unit was defined as: "To cover 1 m^2 of flooring with the optimal performance thickness."

Step 3: As the company is an end-producer for this particular product, the boundaries of the system to be examined is defined as the production process and the use phase. The input-output data supplied by the company took into account the efficiency of the products in coating floors with the optimal thickness.

Step 4 and Step 6: Refer to Fig. 5.9 and Fig. 5.10.

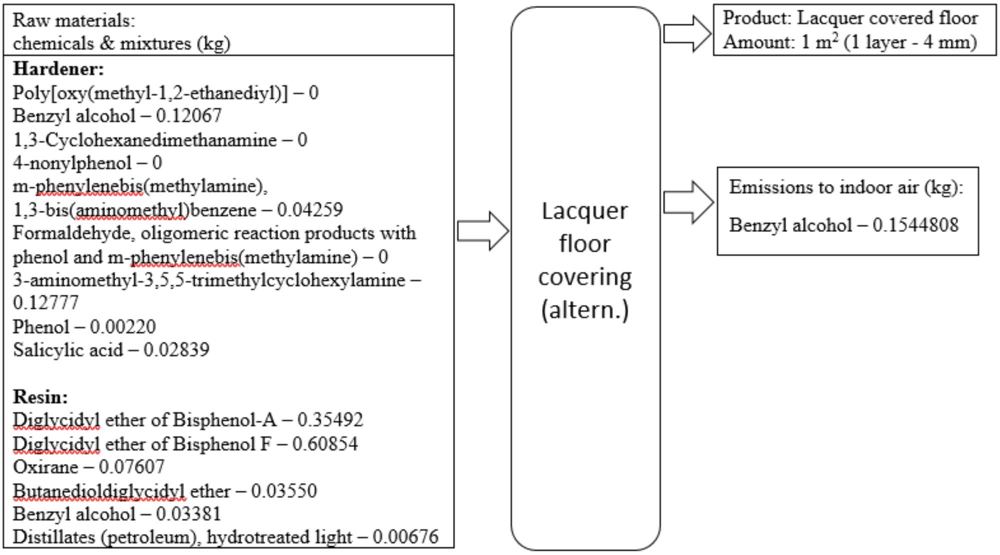

Fig. 5.10. Input-output data for the alternative situation in the production of single layer coated floor in 2016. Only the changed components are shown

Step 5 and Step 7: Production processes for many chemicals were not included in the Ecoinvent database (Ecoinvent, 2017). However, similar chemicals were selected instead of the original ones. The similarity was based on the chemical names (e.g., chemicals including the words 'cyclo' and 'hexane'), chemical properties (e.g., acid), and the molecular composition (i.e., carbon, hydrogen, oxygen, etc., content). Hence; poly[oxy(methyl-1,2-ethanediyl)], 1,3-cyclohexanedimethanamine, 4-nonylphenol, m-phenylenebis(methylamine)(1,3-bis(aminomethyl)benzene), formaldehyde (oligomeric reaction products with phenol and m-phenylenebis(methylamine)), 3-aminomethyl-3,5,5-trimethylcyclohexylamine, salicylic acid, diglycidyl ether of BPA, diglycidyl ether of bisphenol F, oxirane, butanedioldiglycidyl ether, distillates (petroleum)(hydrotreated light) were represented by propylene glycol, cyclohexane, BPA, meta-phenylene diamine, melamine formaldehyde resin, EDTA, benzoic acid, BPA epoxy based vinyl ester resin, melamine formaldehyde resin, alkyl benzene sulfonate, ethylene glycol diethyl ether and light fuel oil, respectively.

Step 8 and Step 9: Step 8 and Step 9 were not necessary. The company had already had its input-outputs normalized to the functional unit.

Step 10: There were no common items to be excluded in the input-output tables between the baseline and the alternative cases. This is due to the company reporting only the implemented changes.

Step 11, Step 12 and Step 13: In Step 11, the data was entered into SimaPro. In Step 12, there was no missing data regarding the emitted substance properties. The results obtained in Step 13 were as shown in Table 5.41.

Table 5.39. Results of the LCA part of the methodology for floor coating case

Damage category	Unit	Floor coating Alternative	Floor coating Baseline
Human Health	DALY	3.92E-5	2.25E-5
Ecosystems	species.yr	1.2E-7	6.53E-8
Resources	$	0.44	0.25

Step 14 and Step 15: Representative life cycle processes of floor coating baseline and alternative cases are listed in Table 5.40 and Table 5.41, respectively.

Table 5.40. Representative life cycle processes of floor coating case classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the baseline situation

Representative life cycle processes and their output amounts						
0.30 MJ Light fuel oil[1]	0.01 kg Ethylene glycol diethyl ether	0.03 kg Alkyl benzene sulfonate, linear	0.05 kg Melamine formaldehyde resin (2)	0.36 kg BPA epoxy-based vinyl ester resin (2)	0.02 kg EDTA	0.02 kg Cyclohexane
0.08 kg Benzyl alcohol (2)	0.08 kg Propylene glycol (2)	0.06 kg Propylene oxide (2)	0.09 kg Benzyl chloride (2)	0.06 kg Benzene	0.14 kg Epoxy resin (2)	0.04 kg BPA powder (2)
0.04 kg Methacrylic acid (2)	0.15 kg Styrene (2)	0.04 kg Melamine (2)	0.05 kg Propylene	0.10 kg Chlorine	0.07 kg Toluene	0.03 kg Phenol (2)
0.03 kg Acetone	0.02 kg Hydrogen cyanide	0.08 kg Hazardous waste incineration	0.04 kg Urea, as N	0.05 kg Ammonia	0.03 kg Cumene	

91 nodes, 40 non-market processes

[1] Light fuel oil lower heating value: 40.6 MJ/kg (Engineering ToolBox, 2013)

Table 5.41. Representative life cycle processes of floor coating case classified into NACE Rev. 2 economic activities (color coded, see Table 5.4) for the alternative situation

Representative life cycle processes and their output amounts						
0.13 kg Ammonia	0.05 kg Melamine formaldehyde resin	0.64 kg BPA epoxy-based vinyl ester (2)	0.13 kg EDTA (2)	0.04 kg Meta-phenylene diamine	0.15 kg Benzyl alcohol (2)	0.04 kg Melamine
0.27 kg Styrene (2)	0.08 kg Methacrylic acid (2)	0.03 kg BPA powder	0.25 kg Epoxy resin (2)	0.07 kg Sodium cyanide (2)	2.15 MJ Steam production	0.07 kg Benzene
0.18 kg Benzyl chloride (2)	0.07 kg Urea, as N	0.03 kg Phenol	0.07 kg Hydrogen cyanide (2)	0.14 kg Toluene	0.12 kg Cement (2)	-0.34 MJ Electricity from hard coal[1]
0.75 MJ Heat from natural gas	0.18 MJ Heat from lignite	0.15 kg Hazardous waste incineration (2)	-0.16 MJ Electricity, nuclear[1]	1.70E-4 MJ Electricity from biogas	-0.01 Clinker[1] (2)	-1.30 kg Digester sludge treatment[1]
1.09 MJ Light fuel oil[2]	-0.17 MJ Hard coal/lignite[3] (2)	0.84 MJ Natural gas[3]	-0.016 m^3 Biogas, anaerobic digestion of manure[1]			

97 nodes, 42 non-market processes

[1] Negative values indicate the deduction of the process from the technosphere (due to the substitution/system expansion method intended to eliminate the co-products in the joint processes as suggested by ISO 14044);

[2] Light fuel oil lower heating value: 40.6 MJ/kg (Engineering ToolBox, 2013);

[3] Upstream fuel operation for some part of the produced electricity (90% plant efficiency assumed)

Step 16: Refer to Table 5.4 in Section 5.1.1.

Step 17: Life cycle accident impacts of the floor coating case can be seen in Table 5.42.

Table 5.42. WE-CFS method results for floor coating case in DALY units

NACE Rev. 2 activity	**Floor coating Baseline situation (years)**	**Floor coating Alternative situation (years)**
C19	4.04E-12	1.46E-11
C20	7.46E-9	5.98E-9
D35	-	1.90E-10
B05	-	3.62E-11
B06	-	1.93E-11
Total:	**7.47E-9**	**6.24E-9**

Step 18, Step 19 and Step 20: The cancer/non-cancer scores of intermediate chemicals concerning the floor coating case can be seen in Table 5.43 and Table 5.44 (refer to Annex II). For the baseline situation, a cancer score of 1.77E-2 and a non-cancer score of 3.15E-2 were obtained. In the alternative situation, a cancer score of 2.77E-2 and a non-cancer score of 8.39E-3 were obtained.

Step 21: Detailed results of the Modified LCIT method for the floor coating case are outlined in Table 5.45 and Table 5.46 (refer to Annex II).

Step 22 and Step 23: Results after normalization and weighting are given in Table 5.47.

Table 5.47. Total normalized and weighted results for floor coating case, excluding modified LCIT 'water emissions', RA and usage/emission amounts

	Simplified LCA			**1.90E-3*Modified LCIT 'air emissions'**			
Situations	**Human Health**	**Ecosystems**	**Resources**	**Human Health**	**Ecosystems**	**WE-CFs**	**Total[1,2]**
Unit	**DALY**	**species.yr**	**$**	**DALY**	**species.yr**	**DALY**	**-**
Baseline	2.25E-5	6.53E-8	0.25	4.29E-8	3.96E-11	7.47E-9	**4.76E-1**
Alternative	3.92E-5	1.20E-7	0.44	3.28E-8	7.65E-11	6.24E-9	**8.44E-1**

[1] Except modified LCIT 'water emissions';

[2] LCIT method results included

For RA, PROC 3 and ERC 8c were adopted. The RA results for the floor coating case are given in Table 5.48.

Table 5.48. Risk assessment result for floor coating case

	Workers RCR (above 1)	**Consumers RCR (above 1)**	**Environment RCRs (above 1)**
Baseline situation	Yes	Yes	Yes (except for terrestrial; man via environment unknown)
Alternative situation	Yes	Yes	No (man via environment unknown)

The usage/emission amounts method results for the floor coating case are listed in Table 5.49 and Table 5.50.

Table 5.49. Usage/emission amounts results for baseline situation of floor coating case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	0.22	0.04	0.01
	Endocrine disruption	0	0	0
	Highly flammable/explosive/reactive	N/A	N/A	0.50
	Carcinogenic/mutagenic	0.03	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	PBT and vPvB (that are missing in LCA)	N/A	N/A	0
	Carcinogenic/mutagenic	0	N/A	N/A

Table 5.50. Usage/emission amounts results for alternative situation of floor coating case

	Hazard type	**Suspected (kg)**	**Animal studies (kg)**	**Known (kg)**
Total usage along life cycle (worker impacts)	*Reprotoxicity*	0.41	0.03	0
	Endocrine disruption	0	0	0
	Highly flammable/explosive	N/A	N/A	0.55
	Carcinogenic/mutagenic	0.03	N/A	N/A
Total emission from company (human health and environmental impacts)	*Reprotoxicity*	0	0	0
	Endocrine disruption	0	0	0
	PBT and vPvB (that are missing in LCA)	N/A	N/A	0
	Carcinogenic/mutagenic	0	N/A	N/A

Evaluation of the results and implementation

The company struggled in finding alternatives that would not include hazardous substances. An alternative was identified; however, the alternative includes BPA in the resin.

If normalization as outlined in Section 2.6 can be applied, the usage/emission amounts method results would yield negligible differences compared to the Simplified LCA results. The baseline situation is preferable in all the aspects except for the local risk to the environment. Due to this, no clear conclusion could be drawn.

A 77% increase in the life cycle environmental impacts was observed.

Many processes were missing from the LCI database, and representative chemicals had to be chosen. However, the choice of these chemicals is not well established, and it was expected to be the source of major uncertainty thus rendering the results almost meaningless for this case. Under these circumstances, the use of the ‘wisdom of the crowds’ effect can be suggested, and only after demonstrating whether it could be shown that it could decrease the errors caused by mistakes due to assessors or missing processes in the databases for this particular product, as in the case of solvents for paints.

5.2. Environmental impact assessment model discussions

To the best of the author's knowledge, there is no existing methodology for the quantification of the impacts of reprotoxic/endocrine disruptor substances, and such issues can only be targeted by evaluating the usage and emission amounts. The usage amounts method addressed the issue of additive effects of reprotoxic/endocrine disruptor substances by considering the usage along the whole supply chain. Neither in the existing frameworks, nor in substitution practices (Subsport, 2016c) is this issue addressed. For example, in the metal sheet priming case, an increase in the use of a suspected reprotoxic substance (toluene) was tolerated due to the assurance from ECHA regarding toluene's safety in industrial setups (ECHA, 2007). This result is very different from similar studies on alternatives to methylene chloride in paint strippers, in which, the conclusion was to exclude alternatives that use toluene (Jacobs *et al*., 2015; Morose *et al*., 2017). Furthermore, in many substitution cases for various products, toluene was substituted based on merely hazard assessment (Subsport, 2016c). The author stresses that the proposed model may consider comprehensive RAs in the decision-making process, while the hazard assessment-based methods overlook this aspect. Due to this dependence of the model results on the risk assessments performed by regulatory bodies, the developed model can yield different outcomes for the different regions of the world. In the case of toluene, the regulatory difference was between California's Proposition 65 (Jacobs *et al*., 2015) and the EU REACH regulation. The only case where reprotoxicity was not an issue was the PU foam production case.

The evaluation of the technical and economic requirements is very similar to many of the already existing alternatives assessment frameworks (Ontario Toxics Use Reduction Program, 2012; IC2, 2013), and this framework structure is stressed to be more appropriate for capturing the life cycle and regulatory aspects of all the potential alternatives, and could be applied without problems in all cases. Unlike in some frameworks (Rossi *et al*. 2011; NRC 2014), the life cycle thinking should be the primary filter for environmental concerns.

The novel important aspects that are covered by the proposed model include systematic and quantitative life cycle thinking for occupational safety and impacts from intermediate chemicals and physical accidents, fugitive and accidental emissions, and reprotoxic/endocrine disruption/PBT/vPvB/physical hazards from chemicals along the supply chain.

Unlike other established frameworks (Rossi *et al*., 2006; Rossi *et al*., 2011; Ontario Toxics Use Reduction Program, 2012; IC2, 2013; NRC, 2014), all the results (except for RA) were based on the functional unit. The use of quantitative methods with their results normalized to the functional unit is more meaningful.

The technical complexity of the methods in use varies from complex (e.g., Simplified LCA) to simple (e.g., usage amounts). This is similar to all the other established frameworks that include LCA (Rossi *et al.*, 2006; Rossi *et al*. 2011; Ontario Toxics Use Reduction Program, 2012; IC2, 2013; NRC, 2014). The adoption of the Simplified LCA was justified by a much lower resource intensity of the method compared to the full LCA (due to the use of generic values) despite the complexity of the method (EEBGUIDE PROJECT, 2012). The same is true for the adoption of the RA. The WE-CFs, LCIT, Modified LCIT, usage/emission amounts methods are relatively less complex. The resource intensiveness of the developed model is low considering its complexity as complex methods are supported by software and use generic values from databases.

The WE-CFs method can be improved by more detailed EU databases and serve as a simpler alternative to very complex modelling-based occupational RA methods applied for widely used products/processes. This would also contribute to obtaining comparable impact results between the LCA and the WE-CFs methods, as concluded by Scanlon *et al*. (Scanlon *et al*., 2015). Besides, the model evaluates the baseline scenario and the alternative scenarios under the same considerations thus overcoming the above mentioned ‘hidden regrettable substitution’. The proposed environmental impact assessment model was able to cover the other above mentioned important issues not just in the company, but also along the supply chain. The proposed model addresses the need for streamlining the substitution process and the subsequently arising issues with double counting (Jacobs *et al*., 2016; Winnebeck and Bawden 2016). These improvements are expected to overcome the almost non-existent application of LCA and other life cycle concerns in practice (Winnebeck and Bawden 2016); that is crucial for a healthy decision on the success of the substitution.

The LCIT method did not produce any results in the fabric bleacher case due to lack of toxicity values regarding the chemicals in use as these chemicals are considered relatively non-toxic.

In the floor coating case, data gaps in LCI caused major problems that can potentially be targeted by the ‘wisdom of the crowds’ effect.

The accuracy of the model can be increased by accounting for more ‘representative processes’. However, the help of a software item is beneficial and necessary from the perspective of resource intensiveness. As the scope of the model is streamlined, the development of a user-friendly software item with automatic extraction of the chemical properties and the amounts from databases and the LCA software would benefit the SMEs and assessors with limited resources (Say *et al*. 2007).

The human and environmental health impacts of nanomaterials and their exposure modelling for incorporation into the chemical alternatives assessment frameworks are expected to be a challenging study area (Walker *et al*. 2015).

From the recycling point of view, what concerns the reduction of hazardous substances in waste streams, the proposed model currently does not offer any solutions.

5.3. Results of the examination of ‘inexpert outcome’ for systematic error in Simplified LCA

The results for the evaluation of systematic errors for company cases described in Section 5.1 are outlined in Table 5.51, Table 5.52, Table 5.53 and Table 5.54.

Table 5.51. Percent difference in impact results for the outcomes of the assessment with maximum number of mistakes (see Section 4.3.2) made by inexpert assessor for fabric bleacher case

Case name (i)	**Mistake type**	**Simplified LCA results**			**$\%_i$ error**			**Ratio (Alternative/Baseline)**	**Ratio for mistake (Alternative/Baseline)**
		Human health (DALY)	**Ecosystem impact (species.y)**	**Resources (USD 2013)**	**Human health**	**Ecosystem impact**	**Resources**		
Fabric bleacher Baseline	-	1.36E-5	2.13E-8	0.06	-			Human health: 2.79 Ecosystem impacts: 2.21 Resources: 1.18	Human health: 2.76 Ecosystem impacts: 2.16 Resources: 1.13
Fabric bleacher Baseline mistake	Systematic (Hydrogen peroxide emission excluded)	1.36E-5	2.13E-8	0.06	0	0	0		
Fabric bleacher Alternative	-	3.79E-5	4.71E-8	0.07	-				
Fabric bleacher Alternative mistake	Systematic (enzyme, EDTA inputs and hydrogen peroxide emission excluded) and random (wrong enzyme)	3.75E-5	4.61E-8	0.06	-1	-2	-4		

Table 5.52. Percent difference in impact results for the outcomes of the assessment with maximum number of mistakes (see Section 4.3.2) made by inexpert assessor for metal sheet priming case

Case name (i)	**Mistake type**	**Simplified LCA results**			**$\%_i$ error**			**Ratio (Alternative /Baseline)**	**Ratio for mistake (Alternative /Baseline)**
		Human health (DALY)	**Ecosystem impact (species.y)**	**Resources (USD 2013)**	**Human health**	**Ecosystem impact**	**Resources**		
Metal sheet priming baseline	-	1.28E-7	2.95E-10	1.35E-3	-			Human health: 0.37 Ecosystem impacts: 0.64 Resources: 1.00	Human health: 1.88 Ecosystem impacts: 1.94 Resources: 2.03
Metal sheet priming baseline mistake	Systematic (Transport excluded), systematic (1-methoxy-2-propanol excluded in inputs)	1.75E-8	7.68E-11	6.20E-4	-86	-74	-54		
Metal sheet priming alternative	-	4.78E-8	1.89E-10	1.36E-3	-				
Metal sheet priming alternative mistake	Systematic (Transport excluded), systematic (NMVOC excluded)	3.29E-8	1.49E-10	1.26E-3	-31	-21	-7		

Table 5.53. Percent difference in impact results for the outcomes of the assessment with maximum number of mistakes (see Section 4.3.2) made by inexpert assessor for polyurethane foam production case

Case name (i)	**Mistake type**	**Simplified LCA results**			**$\%_i$ error**			**Ratio (Alternative /Baseline)**	**Ratio for mistake (Alternative /Baseline)**
		Human health (DALY)	**Ecosystem impact (species.y)**	**Resources (USD 2013)**	**Human health**	**Ecosystem impact**	**Resources**		
PU foam production baseline	-	2.22E-9	6.64E-12	9.44E-6	-			Human health: 0.38 Ecosystem impacts: 0.38 Resources: 1.58	Human health: 0.33 Ecosystem impacts: 0.35 Resources: 1.62
PU foam production baseline mistake	Systematic (2-butoxyethanol excluded)	2.10E-9	6.40E-12	8.37E-6	-5	-4	-11		
PU foam production alternative	-	8.39E-10	2.51E-12	1.49E-5	-				
PU foam production alternative mistake	Systematic (Thiophene excluded)	6.86E-10	2.23E-12	1.36E-5	-18	-11	-9		

Table 5.54. Percent difference in impact results for the outcomes of the assessment with maximum number of mistakes (see Section 4.3.2) made by inexpert assessor for floor coating case

Case name (i)	**Mistake type**	**Simplified LCA results**			**$\%_i$ error**			**Ratio (Alternative /Baseline)**	**Ratio for mistake (Alternative /Baseline)**
		Human health (DALY)	**Ecosystem impact (species.y)**	**Resources (USD 2013)**	**Human health**	**Ecosystem impact**	**Resources**		
Floor coating case baseline	-	2.25E-5	6.53E-8	0.25	-			Human health: 1.74 Ecosystem impacts: 1.84 Resources: 1.79	Human health: 2.02 Ecosystem impacts: 2.01 Resources: 2.01
Floor coating case baseline mistake	Systematic (Missing chemicals excluded)	3.14E-6	7.01E-9	0.03	-86	-89	-90		
Floor coating case alternative	-	3.92E-5	1.20E-7	0.44	-				
Floor coating case alternative mistake	Systematic (Missing chemicals excluded)	6.33E-6	1.41E-8	0.05	-84	-88	-88		

In the case of systematic errors, two cases yielded very high errors, up to 10-fold less than the correct value. Inexpert assessors are not advised to perform the assessments in the case of missing data or a chemical name, as this causes systematic errors. Nonetheless, a statistical method, namely, the ‘wisdom of the crowds’ effect, was proposed to address the data gaps in order to avoid systematic errors (See Section 4.2). Also, suitability of the assessments in case of random errors was examined in the section concerning the ‘wisdom of the crowds’ effect (See Section 4.2).

5.4. Results and discussion for the examination of the ‘wisdom of the crowds’ effect

5.4.1. Results of the qualitative evaluation

As described in Section 4.2, qualitative evaluation involves answering questions regarding the existence of error probability distributions around a mean value, ‘sufficient’ number of independent random selections from these distributions, and aggregation over these independent selections (refer to Table 5.55). The logic behind answering these questions for each specific case is discussed in this section.

For the ‘classifying into economic activities’, the number of all economic activity categories is equal to the number of states and errors expected to be random unless there is a bias towards a specific economic activity more than towards others. ‘Fatal accident determination’ and ‘extent of damage’ both have a two-state discrete distribution with the mode as the correct value. The ‘extent of damage’ contains a systematic error if it is biased towards levels 1 or 2; it is random if it is not biased towards levels 1 or 2. The ‘fatal accident determination’ (despite assuming two-state discrete distribution with the mode as the correct value) is assumed to contain systematic errors due to the system bias as there is a greater number of non-fatal accidents than fatal accidents. Similarly, the ‘probability levels’ have a three-state discrete distribution with the mode as the correct value. For this entity, errors are systematic if biased towards levels 1 or 3; they are random if not biased towards levels 1 or 3.

Similar to the systematic exclusion of entities in the methods as in ‘neglecting missing processes’ due to lack of knowledge, ‘sub-process determination’ gives rise to systematic errors. For ‘sub-process determination’, for inexpert assessors, the correct value is not always positioned at the mode. This is due to the tendency of inexpert assessors to ignore sub-processes that they are not aware of. This is similar to the ‘categorizing into benchmarks’ as inexpert assessors tend to ignore unknown data. All the results are listed in Table 5.55.

Table 5.55. Entities with regards to the existence of error probability distributions around a mean value, ‘sufficient’ number of independent random selections from these distributions, and aggregation over these independent selections.

		Criteria			
Assessment/Entity	**Sub-assessment/ Error details**	**Possible existence of Gaussian/lognormal error probability distributions around a correct value (mode)**	**‘Sufficient’ number of independent selections from these distributions**	**Selections random/ systematic**[2]	**Direct/ indirect**[3] **aggregation over these selections**
LCA inventories	**Measurement**	*Yes*[5]	*?*	*Random*[1]	*Yes*
Simplified LCA inexpert assessor mistakes	**Functional unit/reference flow**	*Yes*	*?*	*Random*	*No*[4]
	Process selection	*Yes*[5]	*?*	*Random*[6]	*Yes*
	Inventory amount	*Yes*[5]	*?*	*Random*	*Yes*
	Neglecting missing process	*No*	*N/A*	*Systematic*	*Yes*
LCIT method	**Functional unit/reference flow**	*Yes*	*?*	*Random*	*No*[4]
	Intermediate flows	*Yes*	*?*	*Random*	*Yes*
	Effect factors	*Yes*	*?*	*Random*[6]	*Yes*
WE-CFs method	**Functional unit/reference flow**	*Yes*	*?*	*Random*	*No*[4]
	Intermediate flows	*Yes*	*?*	*Random*	*Yes*
	Classifying into economic activities	*Yes*[7]	*?*	*Random*[6]	*Yes*
LCRA	**Fatal accident determination**	*Yes*[7]	*?*	*Systematic*	*Yes*
	Sub-process determination	*No*	*N/A*	*Systematic*	*Yes*
	Probability levels	*Yes*[7]	*?*	*Random*[6]	*Yes*
	Extent of damage	*Yes*[7]	*?*	*Random*[6]	*Yes*

Assessment/Entity	Sub-assessment/ Error details	Possible existence of Gaussian/lognormal error probability distributions around a correct value (mode)	‘Sufficient’ number of independent selections from these distributions	Selections random/ systematic [2]	Direct/ indirect [3] aggregation over these selections
GreenScreen®	**Obtaining data**	*No*	*N/A*	*Systematic*	*No* [4]
	Categorizing into benchmarks	*No*	*N/A*	*Systematic*	*No* [4]

[1] As long as the measurement methods/devices do not inherently give rise to systematic errors for the measurement/decision of the amount of the entity;

[2] Systematic errors arise due to bias towards a direction. There is a question to be asked: “Does the correct value (mode) of the distribution for inexpert assessors among all possible distributions have a biased position in the distribution?”;

[3] Here, indirect aggregation means summation of selections after multiplying them with other entities;

[4] Except for the case of using the average of independent repetitions (e.g., average reference flow amount of many assessors);

[5] The error space is assumed to be a lognormal distribution similar to the LCIs that are known to be lognormal (Qin, Suh, 2017);

[6] Unless there is a bias for the correct values in the system towards one direction in the error space;

[7] Non-uniform discrete distribution assumed

5.4.2.Results of the quantitative evaluation

While the obtained results (by using the Recipe Endpoint characterization and damage impact methodologies; refer to Section 4.2) were averaged (by applying arithmetic and geometric averages), the geometric mean exhibited problems with negative (-) and zero (0) values for endpoint characterization impacts. Hence, at first, percentage error progression numbers with ‘odd’ values were excluded (except for the first case). Also, ‘even’ percentage error progression numbers yielded errors for negative (-) values; they were also excluded. Although the results were promising, later it was decided to abandon the negative values altogether due to the introduction of increased uncertainty. By using the ‘=mode()’ function of Microsoft Excel, we would solve the problems with negative values, but we preferred to see how the geometric mean would perform. In addition, as a technical problem, Microsoft Excel gave an error (i.e., -100) for very high roots of some values, hence, they were excluded as well.

The endpoint damage results (with geometric averaging) of the quantitative examination of the Simplified LCA (as performed for solvent-based paints) are presented in Fig. 5.11. As the inexpert assessor results were averaged, the results became more and more accurate, ultimately reaching a stable value.

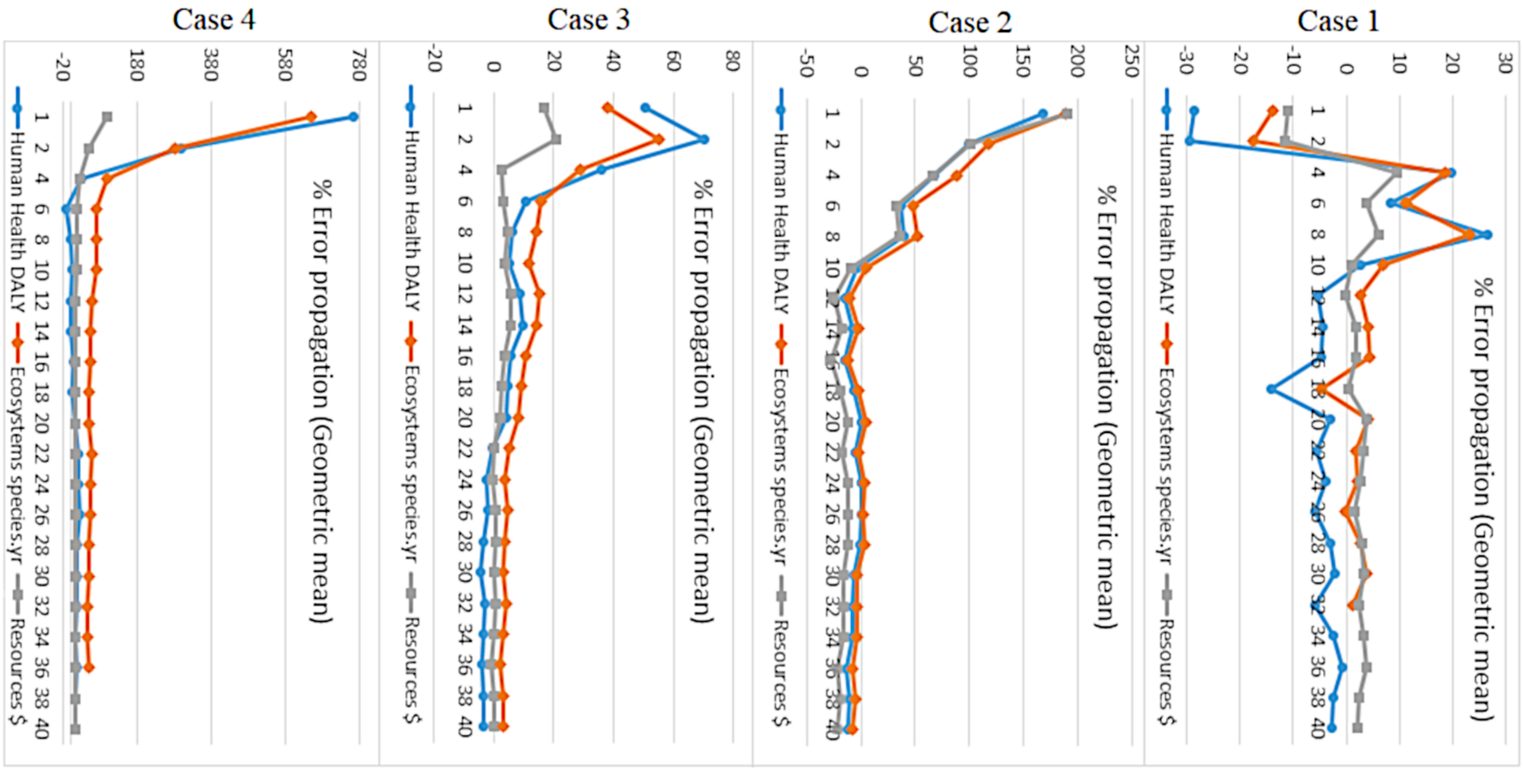

Fig. 5.11. The progression of the percentage error of the geometrically averaged results of independent inexpert assessors from the correct value as the number of inexpert assessors progresses (from 1 to 40). In Cases 1 and 4, ‘ ecosystems’ impact category had technical errors in Excel sheets (i.e., gave ‘ -100’) for assessment numbers over 32 and 36, respectively. These technical errors were excluded from the graphs

The percentage error results of the geometric mean of 40 inexpert assessors for the endpoint damage categories are listed in Table 5.56.

Table 5.56. Percentage error of the geometric mean of 40 inexpert (simulated) assessor results for endpoint damage categories

	Case 1 error (%)	**Case 2 error (%)**	**Case 3 error (%)**	**Case 4 error (%)**
Human health (DALY)	*-2.7*	*-12*	*-3.5*	*12.8*
Ecosystems (species.yr)	*1.3*	*-7.8*	*3.1*	*50.3*
Resources (USD 2013)	*2.2*	*-21.6*	*0.0*	*13.6*

In comparison to the geometric mean, the arithmetic mean yielded higher errors (refer to Fig. 5.12).

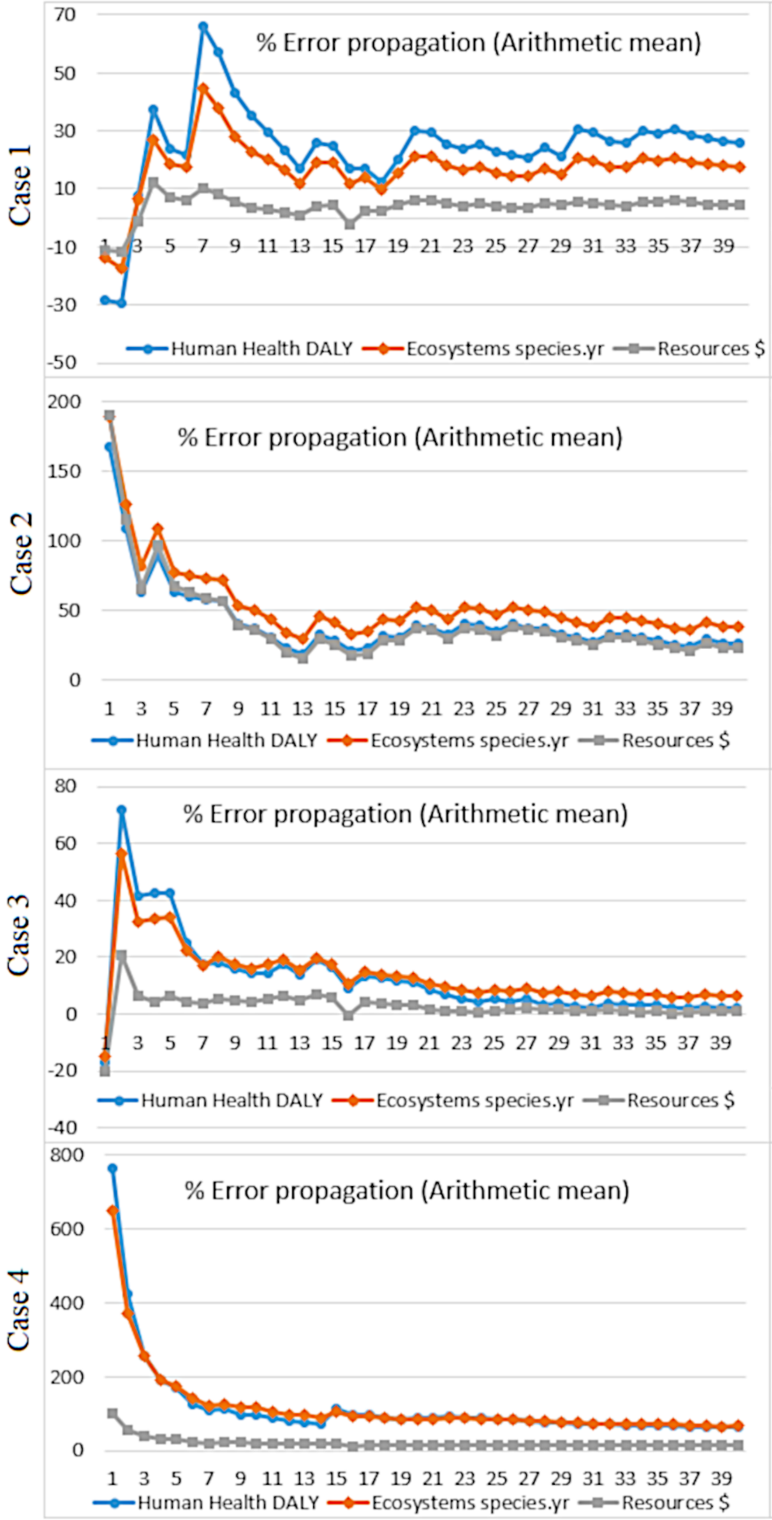

Fig. 5.12. Progression of the percentage error of the arithmetically averaged results of independent inexpert assessors from the correct value as the number of inexpert assessors progresses (from 1 to 40)

5.4.3. Discussion of the results of the ‘wisdom of the crowds’ effect

A ‘sufficient’ number of independent selections depends on the number of variables in the system and on the variance of each variable; hence it is different for each situation (the assessment type, the expertise level of the assessor, etc.).

Further studies in this direction might give an idea about which assessments or which part of the assessments can be performed by inexpert assessors, under which conditions, and which should be left for the experts as they are limited in number. The entities in Table 5.55 with criteria Yes/?/Random/Yes (in that order, according to Table 5.55) or Yes/?/Random/No[4] (in that order, according to Table 5.55) have the potential to deliver the ‘wisdom of the crowds’ effect. They might also help with a more rational planning of the assessment structure so that to exploit this phenomenon in order to reduce errors. For instance, one might prefer performing assessments over the whole life cycle whenever relevant in order to average out the errors instead of conducting local assessments. The results also suggest that performing simplified LCA might be recommended to an inexpert assessor if there is availability of a ‘sufficient’ number of input-output numbers or expertise to balance the lack of the ‘sufficient’ number of input-outputs.

The methods that meet the first three criteria (yes/?/random, in that order, according to Table 5.55) can be further improved in terms of uncertainties if the results from many separate assessors are averaged over. With this in consideration, 12 out of 16 of the entities/sub-assessments showed potential for the ‘wisdom of the crowds’ effect to be present/applied.

The qualitative method was also useful to evaluate the error tendencies for (almost) expert assessors.

Quantitative evaluation of the application of simplified LCA to the solvent-based paint case studies yielded promising results, especially at endpoint damage categories. The damage impact categories showed no negative values (except for 1 inexpert assessment result for ‘ecosystems’ out of 40 assessments and 3 impact categories, i.e., 1 negative out of 120 values in total). In many cases, a very rapid decrease in error occurred, and reasonable accuracy was reached within 10 inexpert assessors. The highest error observed in the ecosystems impact was determined for Case 4; it was a 1.5-fold increase compared to the correct value. It can be stressed that if inexpert assessors had made errors in the amounts of the input-outputs, this number would have increased. However, it is easier to show that the effect would exist in the case of changing amounts than in the case of changing input-output names or regarding the country or technology. In the latter cases, the distribution of the errors is harder to imagine.

Improvement in the accuracy of the results when the geometric average has been used can be used to conclude that the error space is ‘closer’ to be lognormally distributed than normally distributed. This supports many other studies that concluded lognormal distribution in LCIs.

The stabilization away from the correct values either indicates that these LCIs were biased (the systematic positioning of the correct values on the error space due to the bias in the overall system was observed), and/or the number of input-outputs was not sufficient. Although the first explanation is likely as there is a systematic tendency to use less hazardous substances, etc., in the overall system, and it thus can explain the stabilization above the correct values, this still cannot explain the negative errors, such as in Case 2. The latter explanation is more probable and can be improved by having higher input-output numbers.

For endpoint characterization impacts, it was possible to find accurate (comparable to endpoint damage errors) results for most of the impact categories by either using the arithmetic mean or the geometric mean. However, this complicates the application of this technique as deciding on the type of average to be used is not straightforward and needs close examination of the values involved. The endpoint characterization impacts that approach stability from the negative error values yielded better results with the arithmetic mean. This is due to that fact that the geometric mean is not suitable for negative values and also, in some cases, the arithmetic mean combined with an insufficient number of input-output numbers delivered better results (by chance) than the geometric mean by possibly offsetting each other. Hence, for endpoint characterization impacts, both the arithmetic and geometric means are needed depending on the case and the impact category. Further studies are needed to find patterns in the behavior of endpoint characterization errors.

It is a convenient coincidence that the endpoint impacts are both the most affected by the ‘wisdom of the crowds’ effect (due to additional aggregation, hence, more potential cancellation of the errors), and are also the most suitable for inexpert assessors.

As making mistakes around the ‘correct’ process is equivalent to choosing from processes around the ‘correct’ process, the ‘wisdom of the crowds’ effect can also be used to reduce errors due to missing processes in the LCI databases by selecting ‘neighbors’ to the missing process and geometrically averaging the results.

In practice, further examination of the existence of the effect can be based on product categories (e.g., a solvent). For missing chemicals/products/processes (in which the existence of the effect has been proven to be substantial), a single inexpert assessor can perform the assessment by selecting similar sounding chemicals/products/processes multiple times (for solvents, 10 times proved to be enough). Ideally, a word selection software unit (that can select words with common letter combinations) can be utilized.

6. Conclusions

1. State-of-the-art substitution practices are not widespread in terms of evaluation of the life cycle impacts and ignore life cycle concerns for reprotoxic, endocrine disruptor substances, as well as impacts from fugitive/accidental emissions and the workers’ health along the supply chain.

2. The developed environmental impact assessment model for the substitution of hazardous substances while using the life cycle approach was applied in different industrial companies from various industrial branches. The model enabled:

  a. streamlined and harmonized application of environmental impact assessment methods in terms of the scope of impacts and inventory;
  b. evaluation of reprotoxic, endocrine disruptor, bio-accumulative and suspected carcinogen substances along the life cycle;
  c. evaluation of fugitive and accidental emissions along the life cycle;
  d. consideration of the workers' safety along the life cycle;
  e. consideration of the baseline situation.

3. The developed environmental impact assessment model for the substitution of hazardous substances while using the life cycle approach was tested in the four selected industrial company cases:

  a. The *Fabric bleacher* case where, in the alternative situation, life cycle environmental impacts increased by 140%, although a reduction in risk to consumers and a reduction of reprotoxic substances along the supply chain was observed.
  b. The *Metal sheet priming* case where the substitution resulted in 37% reduction in life cycle environmental impacts without any change in local/regional risk. Use of substances with suspected reprotoxic properties was increased, while carcinogenic/mutagenic substances in the supply chain showed a decrease.
  c. The *PU foam production* case where, despite a 42% decrease in the life cycle environmental impacts and a 56% decrease in carcinogenic/mutagenic substances in the supply chain, the use of reprotoxic substances and highly flammable/explosive/reactive substances showed an increase. Emissions of carcinogenic/mutagenic substances from the company were also eliminated.
  d. The *Floor coating* case where life cycle environmental impacts showed a 77% increase. The usage of suspected reprotoxics in the supply chain almost doubled, and the known reprotoxics were eliminated, while carcinogenic/mutagenic substances were reduced by 15%.

The use of highly uncertain normalization factors for the usage/emission amounts method and the incompatibility of the RA method prevented from reaching a sound conclusion in this particular case.

Regulatory differences affect the model outcomes.

4. For inexpert assessors, the proposed impact assessment model can be used in case of no missing data, or if the assessor is bound to benefit from the error reduction method 'wisdom of the crowds' effect. For solvent paints, considerable error reduction was observed at a level of 10 inexpert assessors. For the geometric average of 40 inexpert assessors, in Case 1 and Case 3, the error margin was less than 3.5%, and it was less than 22% for Case 2 and Case 4, except for the 50% error observed for ecosystem impacts in Case 4. Hence, the 'wisdom of the crowds' effect proved to be applicable.

The proposed expert system (harmonized internet system) is necessary for the wider adoption of the proposed environmental impact assessment model by SMEs.

7. Recommendations

A software item to aid the application of the developed environmental impact assessment model (with readily available data and options) will simplify the assessment for the assessors with less expertise. Database improvements also offer major progress towards the reduction of errors and the implementation of the developed environmental impact assessment model by inexpert assessors. Improvement of knowledge on the health effects of reprotoxic substances, endocrine disruptors and nanomaterials is also needed.

Examination of the standard deviation of errors would help to quantify the ‘wisdom of the crowds’ effect. The effect should be examined for other cases in order to identify the range of applicability and thus potentially guide the design of the assessments.

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4. OGUZCAN, S., J. DVARIONIENE. Decision support model for Environmental Impact Assessment of Substitution of Hazardous Substances by Using Life Cycle Approach. 22nd Junior Scientists Conference, Environmental Protection Engineering, Vilnius Gediminas Technical University, 20 March 2019, Vilnius.

Annex I

Chapter 3.

Life cycle inherent toxicity method

Table 3.1. Representative chemicals for the identified organic intermediate flows

Intermediate flow	Representative chemical(s)/substance(s) and CAS No.
Herbicide	100% Glyphosphate (1071-83-6)
Pesticide	50% Estragol (Benzene, 1-methoxy-4-(2-propenyl)-) (140-67-0), 50% Rotenone (83-79-4)
Pyro-oil	0.9% Cresol(s) (1319-77-3), 0.25% Furan (110-00-9), 1.95% Phenol (108-95-2)

Table 3.2. USEtox® effect factors of the identified chemicals (in CTUh (intake) units)

Substance	Cancer (inhalation)	Non-cancer (inhalation)	Cancer (ingestion)	Non-cancer (ingestion)
Glyphosphate	-	0.00410	-	0.00410
Estragol	0.03940	-	0.03940	-
Rotenone	-	0.33438	-	0.33438
Cresol(s)	-	-	-	-
Furan	2.89448	0.32280	2.89448	0.32280
Phenol	-	0.00329	0.00000	0.00329

Table 3.3. Results of life cycle inherent toxicity method for each life cycle stage of the study case

Life cycle stage		Type and amount of intermediate flow		Total (over each life cycle stage) human toxicity impact results per kg intake (CTUh (intake))		% of Total for each disease type and exposure pathway
Agriculture	Herbicide	Glyphosphate	0.00010 kg	Cancer (inh.)	0.00000	0.00
				Non-cancer (inh.)	0.00001	4.35
	Pesticide	Estragol	0.00004 kg	Cancer (inges.)	0.00000	0.00
		Rotenone	0.00004 kg	Non-cancer (inges.)	0.00001	4.35
Transport to pyrolysis		-	-	-	0	0
Overall pyrolysis[1]		-	-	-	0	0
Pyro-oil transport		Cresol(s)	0.00113 kg	Cancer (inh.)	0.00090	50.00
		Furan	0.00031 kg	Non-cancer (inh.)	0.00011	47.83
		Phenol	0.00244 kg	Cancer (inges.)	0.00090	50.00
				Non-cancer (inges.)	0.00011	47.83
Biochar transport		-	-	-	0	0
Electricity		Cresol(s)	0.00113 kg	Cancer (inh.)	0.00090	50.83
		Furan	0.00031 kg	Non-cancer (inh.)	0.00011	47.83
		Phenol	0.00244 kg	Cancer (inges.)	0.00090	50.00
				Non-cancer (inges.)	0.00011	47.83

[1] 'Overall pyrolysis' by assumption includes 'Drying', 'Grinding' and their upstream processes as in Fig. 3.2 (color-coded as in Fig. 3.2).

Table 3.4. Classification of the processes within the defined scope into industry (economic) activity branches (Eurostat, 2008).

Process/product name	**NACE Rev. 2 classification**
Rhizomes	A01 – Crop and animal production, hunting and related service activities
Fertilizer	C20 – Manufacture of chemicals and chemical products
Herbicide	C20 – Manufacture of chemicals and chemical products
Pesticide	C20 – Manufacture of chemicals and chemical products
Biomass cultivation[1]	A01 – Crop and animal production, hunting and related service activities
Transport (truck)	H49 – Land transport and transport via pipelines
Overall pyrolysis[2]	C19 – Manufacture of coke and refined petroleum products
Electricity production	D35 – Electricity, gas, steam and air conditioning supply
Heat from fuel oil	D35 – Electricity, gas, steam and air conditioning supply
Natural gas burning/supply	D35 – Electricity, gas, steam and air conditioning supply
Pipeline transport	H49 – Land transport and transport via pipelines
Petroleum extraction	B06 – Extraction of crude petroleum and natural gas
Petroleum refinery	C19 – Manufacture of coke and refined petroleum products
Diesel	C19 – Manufacture of coke and refined petroleum products
Hard coal	B05 – Mining of coal and lignite
Natural gas	B06 – Extraction of crude petroleum and natural gas

[1] 'Biomass cultivation' includes 'Baling', 'Planting', 'Plowing', 'Harrowing', 'Distribution' and 'Harvesting' as seen in Fig. 3.2.

[2] 'Overall pyrolysis' by assumption includes 'Drying' and 'Grinding' as seen in Fig. 3.2.

WE-CFs method

Years of Life Lost due to fatal accidents per industry sector (r) (Scanlon *et al.*, 2013) (Eq. 4.15):

$$YLL_r = \sum_{a=1}^{M_a} \sum_{s=1}^{2} N_{a,s,r} \cdot L_{a,s} \; ; \qquad \text{(Eq. 4.15)}$$

Here, a is the age strata, M_a is the total number of age strata, and s is sex. In the study by Scanlon *et al.* (2015), M_a has been taken to be 9. In the current study, it is taken to be 3 (see Eq. 4.16).

The data necessary for the calculation of YLL_r was found on the Eurostat website (Eurostat HSW, 2017) under the dataset "Accidents at work by sex, age, severity, NACE Rev. 2 activity and workstation." The dataset was segmented as 'sex', 'age class', 'severity' (set to 'fatal'), 'NACE R2 activity', 'workstation' (set to 'total'), geopolitical entity (set to 'EU-28'), 'unit of measure' (set to 'number'), and 'time' (set to '2014').

However, NACE Rev. 2 activities were not detailed (i.e., they did not involve subsectors). To improve this, another dataset (“Fatal Accidents at work by NACE Rev. 2 activity”) from Eurostat database (Eurostat HSW, 2017) have been used to weigh the fatality of different subsectors (for EU-28 and for the year 2014). In other words, $N_{a,s,r,sub}$ values for industrial subsectors have been derived from sector fatality data (that contains age and sex information, but no information about the subsectors) by using the additional information on the fatal accident counts for a given subsector (see Table 3.14 for the coefficients used). All the data, unless mentioned otherwise, are for the year 2014 and for EU-28 region.

The minimum and maximum working ages are assumed to be 15 and 65, respectively.

$L_{a,s}$ values have been calculated for each ‘age class’ and ‘sex’ in Table 3.12.

Table 3.12. $L_{a,s}$, in years, for each ‘age class’ and ‘sex’

	Less than 25 (15 to 24)	25 to 54	More than 55
Female	(82.4 – 20)	(82.4 – 40)	(82.4 – 60)
Male	(76.6 – 20)	(76.6 – 40)	(76.6 – 60)

$N_{a,s,n}$ values are shown in Table 3.13.

Table 3.13. $N_{a,s,r}$ values

Sector	**Sex**	**Numbers per age group**		
		15 to 24	**25 to 54**	**More than 55**
A – Agriculture, forestry and fishing	Female	1	13	12
	Male	31	275	200
B – Mining and quarrying	Female	0	1	1
	Male	2	58	10
C – Manufacturing	Female	0	13	6
	Male	34	372	149
D – Electricity, gas, steam and air conditioning supply	Female	0	0	0
	Male	1	23	5
H – Transportation and storage	Female	3	12	7
	Male	20	410	174

By using the database (Eurostat HSW, 2017) sections (“Accidents at work by sex, age, severity, NACE Rev. 2 activity and workstation” and “Fatal Accidents at work by NACE Rev. 2 activity”), YLL_r’s have been calculated for each industry sector involved in the pyro-oil case (see Table 3.4). The formula has been modified as follows (Eq. 4.16):

$$YLL_{r,sub} = \sum_{a=1}^{3} \sum_{s=1}^{2} N_{a,s,r} . \frac{f_{r,sub}}{f_r} . L_{a,s} \; ; \qquad \text{(Eq. 4.16)}$$

Here, $f_{r,sub}$ is the fatal accident counts in subsector ‘r,sub’, and f_r is the fatal accident counts in sector r.

$f_{r,sub}/f_r$ values are shown in Table 3.14.

Table 3.14. Subdivision coefficients for each subsector ($f_{r,sub}/f_r$ values)

Subsector	A01	B05	B06	C19	C20	D35	H49
$f_{r,sub}/f_r$ values	377/542	33/72	5/72	1/578	38/578	29/29	506/627

Example calculation of Years of Life Lost due to fatal accidents as applied for 'A01 – Crop and animal production, hunting and related service activities' (as a subsector of 'A – Agriculture, forestry and fishing') by using Eq. 4.17:

$$YLL_{A01} = \sum_{a=1}^{3} \sum_{s=1}^{2} N_{a,s,A} \cdot \frac{f_{A01}}{f_A} \cdot L_{a,s} \qquad \text{(Eq. 4.17)}$$

The weighting factor (f_{A01}/f_A) for subsector A01 is 377/542 (see Table 3.14), hence:

=1*(377/542)*(82.4 – 20)+13*(377/542)*(82.4-40)+12*(377/542)*(82.4-60) +275*(377/542)(76.6-40)+200*(377/542)(76.6-60)+31*(377/542)(76.6-20)= 11144.45 years

Table 3.15 shows the results of YLL calculation for each economic activity by using Tables 3*, A3, A4 and Eq. 4.16.

Table 3.15. YLLs for each economic activity (sub-sectors)

Economic activity	A01	B05	B06	C19	C20	D35	H49
YLL (years)	11144.45	1130.62	171.31	32.35	1229.32	981.40	16042.86

The formulas for the calculation of YLDs for non-fatal accidents required more detailed information, however, this data was not available for the EU-28 region. Despite this difficulty, on the Eurostat (Eurostat HSW, 2017), a dataset named "Accidents at work by days lost and NACE Rev. 2 activity" on the 'work days lost due to accidents' was found to be useful for this purpose. As neither the nature of the injury, nor the age of incidence or the sex information were presented, weightings for injuries based on the report of WHO on disability weights (WHO, 2004) applied only as based on the duration of work days lost, i.e., as based on the assumption that "the longer the duration, the more serious the injury is". Another assumption was "work days lost=days lost" (i.e., work=daily activities in life). Averaged over injury type, short-term (treated) disability weight equaled 0.2256, and long-term (treated) disability weight ('burns <20%' and 'injured nerves' excluded) equaled 0.3082 (W_S values in Eq. 4.18). For the time spent away from work for less than 183 days – as workers were able to recover and turn back to their occupations – the average short-term disability weight was adopted.

YLDs were simply calculated by the following equation (Eq. 4.18):

$$YLD_{r,sub} = \sum_S N_{S,r,sub} \cdot D_S \cdot W_S \,; \qquad \text{(Eq. 4.18)}$$

here, W_S is the disability weight per each day's lost strata S, D_S is the average days lost per each 'days lost' strata S, and $N_{S,r,sub}$ is the number of incidents in each sub-sector and the 'days lost' strata. Table 3.16 and Table 3.17 show the values of $N_{S,r,sub}$ as extracted from the dataset "Accidents at work by days lost and NACE Rev. 2 activity," and the D_S values, respectively.

Table 3.16. Number of incidents in each sub-sector and 'days lost' strata ($N_{S,r,sub}$ values)

Economic activity **Days lost strata**	A01	B05	B06	C19	C20	D35	H49
4-6 days	11408	185	68	54	1353	611	19906
7-13 days	19508	436	64	101	2443	1131	22687
14-20 days	12271	411	86	79	1294	681	14104
21 days-1 month	10849	472	44	77	989	537	12791
1-3 months	19395	1208	80	126	1763	1015	22633
3-6 months	4824	748	29	57	461	354	7484
More than 183 days	7232	131	12	46	405	195	5741

Table 3.17. Average days lost per each 'days lost' strata (D_S values)

Days lost strata	4–6 days	7–13 days	14–20 days	21 days– 1 month	1–3 months	3–6 months	More than 183 days
D_S (days)	5	10	17	25.5	60	135	13906.5[1]

[1] Average life expectancy over sexes was taken to be 79.6 years

As explained, W_S values were taken to be 0.2256 and 0.3082 for below 183 days and for above 183 days, respectively. Table 3.18 shows the results of YLD (weighted) calculation (by using these weights, Table 3.16, Table 3.17, and Eq. 4.18 were derived) for each economic activity.

Table 3.18. YLDs (weighted) for each economic activity (sub-sectors)

Economic activity	A01	B05	B06	C19	C20	D35	H49
YLD (weighted) ('183 days or more' excluded)	1577.54	122.24	7.59	12.26	152.31	91.68	2015.35
YLD (weighted) ('183 days or more' included)	86498.72	1660.49	148.50	552.42	4908.00	2381.45	69428.60
% contribution of '183 days or more' strata to YLD	5383%	1258%	1857%	4406%	3122%	2498%	3345%

However, due to the huge uncertainty caused by the strata '183 days or more', only short-term (i.e., with the strata '183 days or more' excluded) injuries were considered in the study results. Hence, WE_DALYs were calculated as the sum of YLLs and YLDs for each sub-sector (see Table 3.19).

Table 3.19. Gross WE_DALYs per sub-sector

Economic activity	A01	B05	B06	C19	C20	D35	H49
Gross WE_DALY (years)	12721.99	1252.86	178.90	44.61	1381.63	1073.08	18058.21

Production amounts (Table 3.5) are extracted from Eurostat databases.

Table 3.5. Production amounts for each sub-sector for the EU-28 region in 2014.

Economic activity	A01[1]	B05[2]	B06[3]	C19[4]	C20[5]	D35[6]	H49[7]
Production amount	5,14597E+11 kg	5,95153E+12 MJ	7,76082E+12 MJ	3,34685E+12 MJ	3,259E+11 kg	1,46548E+13 MJ	1,72668E+15 kg*km

[1] Crops: Cereals for the production of grain (including seed), Dry pulses and protein crops for the production of grain (including seed and mixtures of cereals and pulses), Industrial crops, Plants harvested green from arable land, Fresh vegetables (including melons) and strawberries, Permanent crops for human consumption, Fruits, berries and nuts (excluding citrus fruits, grapes and strawberries), and Citrus fruits. The missing information for year 2014 was completed as follows: if the amount for both adjacent years was available, we averaged them; if neither value was available, we took the value of the closest year to 2014 while prioritizing the more recent years. Dataset: “Crop statistics (from 2000 onwards)” (Eurostat AP, 2017).

The mass of livestock population (bovine, sheep, goat, pig) is added to the agricultural primary production. Average animal weights were used (85 kg for sheep, 910 kg for a bovine, 30 kg for a goat, and 90 kg for a pig) to convert population numbers into mass units (Agriculture and Horticulture Development Board [AHDB], 2015; McGregor, 2007; Agrawal *et al.*, 2014; Felius, 1995). Dataset: “Bovine/Goats/Equidae/Sheep/Pig population-annual data” (Eurostat AP, 2017).

[2] Coal: Anthracite, Coking coal, Other Bituminous Coal, Sub-bituminous coal and Lignite/Brown Coal. Dataset: “Simplified/complete energy balances – annual data (nrg_100a)” (Eurostat ES, 2017).

[3] Crude petroleum: Crude oil (without NGL) and Natural gas liquids. Dataset: “Simplified/complete energy balances – annual data (nrg_100a)” (Eurostat ES, 2017).

[4] Coke production amounts (Terajoules) were calculated by the amount of coal (coking coal) primarily produced to be used in the coke production, assuming 65% yield coal to coke (Coaltech, 2017), and similar energy content per weight of coal and coke (Food and Agriculture Organization of the United Nations [FAO], 2017). Datasets: “Simplified/complete energy balances – annual data (nrg_100a)” and “Primary production – all products – annual data (nrg_109a)” (Eurostat ES, 2017).

[5] Dataset: “Production and consumption of chemicals by hazard class (env_chmhaz)” (Eurostat CH, 2017).

[6] ‘Electrical energy available for final consumption’, ‘Electricity used for electric boilers’ (steam) and ‘Gas primary production’ are summed up (air conditioning

excluded). Dataset: “Simplified/complete energy balances – annual data (nrg_100a)” and “Primary production – all products – annual data (nrg_109a)” (EU ES, 2017).

[7]‘Total-total transport’ is chosen. Dataset: “Summary of annual road freight transport by type of operation and type of transport (1 000 t, Mio Tkm, Mio Veh-km) [road_go_ta_tott]” (Eurostat T, 2017)

Hence, WE_DALYs (Table 3.6) are calculated by dividing the values given in Table 3.19 for each sector with the values listed in Table 3.5.

Table 3.6. WE_DALYs for each sub-sector

Economic activity	A01	B05	B06	C19	C20	D35	H49
WE_DALY	2.47222172E-8	2.1051054E-10	2.3051688E-11	1.3328933E-11	4.23942927E-9	7.3223715E-11	1.0458336E-11

Table 3.7. WE_DALY impact scores for each process

Life cycle stage	**Process**	**NACE Rev. 2**	**Output amount from processes**	**WE_DALY score**	**% of total**	**% of total for life cycle stages**
Agriculture	Rhizomes	A01	0.00044 kg	1.09E-11	0.09	90.68
	Fertilizer	C20	0.00386 kg	1.64E-11	0.13	
	Herbicide	C20	0.00010 kg	4.24E-13	0.00	
	Pesticide	C20	0.00008 kg	3.39E-13	0.00	
	Biomass cultivation[1]	A01	0.46296 kg	1.15E-8	90.44	
	Diesel[2]	C19	0.19896 MJ	2.65E-12	0.02	
Transport to pyrolysis	Transport (truck)	H49	23.14815 kg*km	2.42E-10	1.91	2.03
	Diesel[2]	C19	1.13838 MJ	1.52E-11	0.12	
Overall pyrolysis[3]	Pyrolysis[4]	C19	2.50000 MJ	3.33E-11	0.26	4.77
	Pipeline transport	H49	40.12075 kg*km	4.20E-10	3.32	
	Heat from fuel oil	D35	0.77341 MJ	5.66E-11	0.45	
	Petroleum extraction	B06	1.04172 MJ	2.40E-11	0.19	
	Petroleum refinery	C19	0.86036 MJ	1.15E-11	0.09	
	Hard coal	B05	0.09326 MJ	1.96E-11	0.16	
	Natural gas extraction	B06	0.39208 MJ	9.04E-12	0.07	
	Natural gas burning/supply	D35	0.39208 MJ	2.87E-11	0.23	
Pyro-oil transport	Transport (truck)	H49	18.75000 kg*km	1.96E-10	1.55	1.59
	Diesel[2]	C19	0.33820 MJ	4.51E-12	0.04	
Bio-char transport	Transport (truck)	H49	4.16667 kg*km	4.36E-11	0.34	0.35
	Diesel[2]	C19	0.11226 MJ	1.50E-12	0.01	
Electricity	Electricity production	D35	1.00000 MJ	7.32E-11	0.58	0.58

[1] ‘Biomass cultivation’ includes ‘Baling’, ‘Planting’, ‘Plowing’, ‘Harrowing’, ‘Distribution’ and ‘Harvesting’ as seen in Fig. 3.2;

[2] Diesel density: 0.8375 kg/L; Diesel fuel heating value: 42.96 MJ/kg;

[3] ‘Overall pyrolysis’ by assumption includes ‘Drying’, ‘Grinding’ and their upstream processes as in Fig. 3.2;

[4] Heating value of pyro-oil: 20 MJ/kg

Table 3.8. Complete inventory table of dangerous situations and related accidents, and the risk level assessment

Life cycle stage	**Process/ Operation**	**Sub-operation**	**Dangerous situation**	**Accident**	**Means of control**		**Things needed for accident to happen**	**p**[2]	**E**[3]
					Protection	**Prevention**			
Agriculture	Rhizomes	-	-	-	-	-	-	-	-
	Fertilizer	Storage	Ammonium nitrate	Explosion-fire	Alarms, protective equipment, equipment maintenance	Zone separation, Training, etc.	Alarm or equipment failure AND spark	1	2
	Herbicide	-	-	-	-	-	-	-	-
	Pesticide	-	-	-	-	-	-	-	-
	Biomass cultivation	Plowing	Tractor	Crush worker	-	Safe stop procedure	Procedure failure AND person on trajectory	1	1
		Planting	Tractor	Crush worker	-	Safe stop procedure	Procedure failure AND person on trajectory	1	1
		Baling	Tractor	Crush worker	-	Safe stop procedure	Procedure failure AND person on trajectory	1	1
			Bale fall	Crush worker	-		Falling bale AND person on trajectory	1	1
		Harrowing	Tractor	Crush worker	-	Safe stop procedure	Procedure failure AND person on trajectory	1	1
		Distribution	-	-	-	-	-	-	-
		Harvesting	Combine Harvester	Crush worker	-	Safe stop procedure	Procedure failure AND person on trajectory	1	1
	Diesel	Storage	Diesel leakage	Explosion-Fire	-	Spark prevention	Leakage AND prevention failure	1	1
	Transport (truck)	Driving	Road traffic	Traffic accident	-	-	Many independent events	3	2

Life cycle stage	Process/ Operation	Sub-operation	Dangerous situation	Accident	Means of control		Things needed for accident to happen	p[2]	E[3]
					Protection	Prevention			
Transport to pyrolysis	Diesel	Storage	Diesel leakage	Explosion-Fire	-	Spark prevention	Leakage AND prevention failure	1	1
Overall pyrolysis[1]	Pyrolysis	Liquid Storage	Leakage	Fire	Firefighting	Spark prevention	Leakage AND spark AND firefighting failure	1	1
		Pyrolysis plant	Leakage	Fire	Firefighting	Spark prevention	Leakage AND spark AND firefighting failure	1	1
			Gas leakage	Explosion	-	Gas detection, spark prevention	Gas detection AND spark prevention failure	1	1
			Char dust airborne	Explosion	-	Dust detection	Dust detection failure	2	1
	Pipeline transport	Pipeline flow	Leakage	Fire	-	Maintenance	Maintenance failure AND spark	1	2
	Heat from fuel oil	Storage	Leakage	Fire	-	Spark prevention	Leakage AND prevention failure	1	1
	Petroleum extraction	Preoperational	Helicopter transport of personnel	Helicopter Crash	Protective equipment (lifejacket, etc.)	Pilot training, helicopter maintenance, weather forecast, etc.	(Pilot failure OR maintenance fail OR protective equipment fail OR weather forecast fail, etc.) AND (protective equipment fail)	1	2

Life cycle stage	Process/ Operation	Sub-operation	Dangerous situation	Accident	Means of control		Things needed for accident to happen	p[2]	E[3]
					Protection	Prevention			
			Platform underwater maintenance	Diving accident (Stroke, drowning, being stuck)	-	Medical check-up, co-diving, training	Procedure failure AND (stroke OR drowning OR being stuck)	1	1
		Drilling	Pressure build up	Mud volcano	-	-	Pressure build up	2	1
			Drilling to a gas pocket	Explosion-fire	-	-	Gas pocket AND spark	1	2
		Collection	Severe weather, floater fail, platform leg fail	Capsize platform	-	-	Severe weather AND weak platform	1	1
			Collision of mobile trailer and drilling platform	Fire	Signaling devices on the platform	-	Signaling device failure AND collision danger	1	1
			Maintenance work on installations (metal tools: spark or static electricity)	Explosion-fire	-	Fire permit, shut down of equipment during maintenance	Spark AND procedure failure	1	2
			H_2S release	Inhalation	Detectors	-	Detector fail	2	1

Life cycle stage	Process/ Operation	Sub-operation	Dangerous situation	Accident	Means of control		Things needed for accident to happen	p[2]	E[3]
					Protection	Prevention			
		Storage	Human intervention	Explosion-fire	Specific instructions	-	Lack of rules AND human negligence	1	2
	Petroleum refinery	Storage	Leakage of distillates	Explosion-Fire	-	Spark prevention	Leakage AND prevention failure	1	2
	Hard coal	Storage	Airborne dust	Explosion-fire	-	Dust detection, spark prevention	Dust detection failure AND spark	1	2
	Natural gas extraction	Storage	Gas leakage	Explosion	-	Gas detection, spark prevention	Gas detection AND spark prevention failure	1	1
	Natural gas burning/supply	Pipelines	Gas leakage	Explosion	-	Gas detection, spark prevention	Gas detection AND spark prevention failure	1	1
Pyro-oil transport	Transport (truck)	Driving	Pyro-oil leakage	Fire	-	-	Puncture of the vessel AND spark	1	2
			Road traffic	Traffic accident	-	-	Many independent events	3	2
	Diesel	Storage	Diesel leakage	Explosion-Fire	-	Spark prevention	Leakage AND prevention fail	1	1
Bio-char transport	Transport (truck)	Driving	Road traffic	Traffic accident	-	-	Many independent events	3	2
	Diesel[2]	Storage	Diesel leakage	Explosion-Fire	-	Spark prevention	Leakage AND prevention failure	1	1
Electricity production	Electricity production	Transmission of electricity	Isolation failure	Exposure to high voltage	Isolation equipment	Maintenance	Isolation failure AND maintenance failure	1	1

[1] 'Overall pyrolysis' by assumption includes 'Drying', 'Grinding' and their upstream processes as shown in Fig. 3.2;
[2] Probability level of occurrence;
[3] Extent of the level of damage

Table 3.9. Classes of risk for each sub-operation/sub-process, classified as described in Fig. 3.1 by using Table 3.8.

Life cycle stage	Process/ Operation	Sub-operation/ Sub-process	Accident	p	E	Risk class
Agriculture	Rhizomes	-	-	-	-	-
	Fertilizer	Storage	Explosion-fire	1	2	2
	Herbicide	-	-	-	-	-
	Pesticide	-	-	-	-	-
	Biomass cultivation	Plowing	Crush worker	1	1	1
		Planting	Crush worker	1	1	1
		Baling	Crush worker	1	1	1
			Crush worker	1	1	1
		Harrowing	Crush worker	1	1	1
		Distribution	-	-	-	-
		Harvesting	Crush worker	1	1	1
	Diesel	Storage	Explosion-Fire	1	1	1
Transport to pyrolysis	Transport (truck)	Driving	Traffic accident	3	2	3
	Diesel	Storage	Explosion-Fire	1	1	1
Overall pyrolysis[1]	Pyrolysis	Liquid Storage	Fire	1	1	1
		Pyrolysis plant	Fire	1	1	1
			Explosion	1	1	1
			Explosion	2	1	2
	Pipeline transport	Pipeline flow	Fire	1	2	2
	Heat from fuel oil	Storage	Fire	1	1	1

Life cycle stage	**Process/ Operation**	**Sub-operation/ Sub-process**	**Accident**	**p**	**E**	**Risk class**
	Petroleum extraction	Preoperational	Helicopter Crash	1	2	2
			Diving accident (Stroke, drowning, being stuck)	1	1	1
		Drilling	Mud volcano	2	1	2
			Explosion-fire	1	2	2
		Collection	Capsize platform	1	1	1
			Fire	1	1	1
			Explosion-fire	1	2	2
			Inhalation	2	1	2
		Storage	Explosion-fire	1	2	2
	Petroleum refinery	Storage	Explosion-Fire	1	2	2
	Hard coal	Storage	Explosion-fire	1	2	2
	Natural gas extraction	Storage	Explosion	1	1	1
	Natural gas burning/supply	Pipelines	Explosion	1	1	1
Pyro-oil transport	Transport (truck)	Driving	Fire	1	2	2
			Traffic accident	3	2	3
	Diesel	Storage	Explosion-Fire	1	1	1
Bio-char transport	Transport (truck)	Driving	Traffic accident	3	2	3
	Diesel[2]	Storage	Explosion-Fire	1	1	1
Electricity production	Electricity production	Transmission of electricity	Exposure to high voltage	1	1	1

Table 3.10. LCRA scores per life cycle without any weighting applied

Life cycle stage	Agriculture	Transport to pyrolysis	Overall pyrolysis	Pyro-oil transport	Bio-char transport	Electricity production
LCRA score	1.125	2	1.5	2	2	1
% of total score	11.7	20.8	15.6	20.8	20.8	10.4

Annex II

Table 5.6. LCIT method worker health results for baseline situation of fabric bleacher case

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
Diesel	0.03	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		

Table 5.7. LCIT method worker health results for alternative situation of fabric bleacher case

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
Ethylene dichloride	1.90E-3	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
EDTA	0.01	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Diesel	0.02	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Ethylene diamine	1.70E-3	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		

Table 5.8. Modified LCIT method results for baseline situation of fabric bleacher case

Intermediate chemical/ (release compartment)	Amount (kg)	LCA ReCiPe Endpoint (E)- Human impacts (DALY)	LCA ReCiPe Endpoint (E)- Ecological impacts (species.yr)
Sodium Chloride (water)	0.21	x	x
Diesel/‘petroleum distillate’(air)	0.03	x	x
Total	**0.24**	**x**	**x**

Table 5.9. Modified LCIT method results for alternative situation of fabric bleacher case

Intermediate chemical/(emission compartment)	**Amount (kg)**	**LCA ReCiPe Endpoint (E)-Human impacts (DALY)**	**LCA ReCiPe Endpoint (E)-Ecological impacts (species.yr)**
Sodium Chloride (water)	0.26	x	x
EDTA (water)	0.01	x	3.99E-13
Ethylene diamine (air)	1.70E-3	x	7.25E-12
Hydrogen cyanide (air)	3.20E-3	5.76E-8	1.48E-9
Diesel/‘petroleum distillate’ (air)	0.02	x	x
Ethylene dichloride/‘Ethane, 1,2-dichloro-’ (air)	1.90E-3	2.25E-8	3.00E-13
Sodium cyanide/‘cyanide compounds’(water)	5.40E-3	x	x
Total	**0.30**	**8.01E-8**	**1.49E-9**

Table 5.14. Inventory of (main) chemicals used in the line of cleaning and priming (in 2015).

Product	Composition	CAS	Composition, %	Hazard classes
Hempel's Liquid 99 751	Propan-2-ol	67-63-0	>=50-<75	Flam. Liq. 2, Skin Irrit. 2, STOT SE 3
	Zinc chloride	7646-85-7	>=0.1-<0.25	Acute Tox. 4, Skin corr 1B, Eye Dam. 1, STOT SE 3, Aquatic Acute 1, Aquatic Chronic 1
Shopprimer ZS 15899	Zinc powder	7440-66-6	>=35-<50	Aquatic Acute 1, Aquatic chronic 1
	Butan-1-ol	71-36-3	>=10-<15	Flam Liq. 3, Acute Tox. 4, Skin Irrit. 2, Eye Dam. 1, STOT SE 3,
	Xylene	1330-20-7	>=10-<12.5	Flam Liq. 3, Acute Tox. 4, Skin Irrit. 2
	Ethylbenze-ne	100-41-4	>=1-<3	Flam Liq. 2, Acute Tox. 4, STOT RE 2, Asp. Tox. 1
	Zinc oxide	1314-13-2	>=0.25-<2.5	Aquatic Acute 1, Aquatic Chronic 1
'THINNER 2'	Propan-2-ol	67-63-0	>=35-<50	Flam. Liq. 2, Skin Irrit. 2, STOT SE 3
	Toluene	108-88-3	>=35-<50	Flam Liq. 2, Skin Irrit. 2, Repr. 2, STOT SE 3, STOT RE 2, Asp. Tox. 1
	Xylene	1330-20-7	>=12-<20	Flam Liq. 3, Acute Tox. 4, AcuteTox.4, Skin Irrit. 2
	Ethylbenze-ne	100-41-4	>=3-<7	Flam Liq. 2, Acute Tox. 4, STOT RE 2, Asp. Tox. 1,
	Solvent naphtha light aromatic	64742-95-6	>=5-<7	Flam. Liq. 3, Acute Tox. 4, Skin Irrit. 2, Eye Irrit. 2, STOT SE 3, Asp. Tox. 1, Aquatic Chronic 2
'THINNER 1'	1-metoxy-2-propanol	107-98-2	>=35-<50	Flam. Liq. 3, STOT SE 3
	Xylene	1330-20-7	>=35-<50	Flam. Liq. 3, Acute Tox. 4, Acute Tox.4, Skin Irrit. 2
	Ethylbenzene	100-41-4	>=7-<10	Flam. Liq. 3, Acute Tox. 4, STOT RE 2, Asp. Tox. 1
	2-metoxypropanol	1589-47-5	<0.3	Flam. Liq.3, Skin Irrit. 2, Eye Dam 1, Repr. 1B, STOT SE 3

Table 5.19. LCIT method worker health results for baseline situation of metal sheet priming case

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
Ethylene	8.00E-5	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Diesel	7.98E-4	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Methanol	4.80E-4	Inhalation	-	Inhalation	5.08E-04	-	4.88E-7
		Ingestion	-	Ingestion	5.08E-04		
Propylene oxide	1.75E-3	Inhalation	1.20E-02	Inhalation	2.31E-01	7.18E-5	8.09E-4
		Ingestion	2.90E-02	Ingestion	2.31E-01		
Benzene	3.20E-4	Inhalation	1.47E-02	Inhalation	3.72E-03	9.41E-6	2.38E-6
		Ingestion	1.47E-02	Ingestion	3.72E-03		
Propylene	1.33E-3	Inhalation	0	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Propylene glycol monomethyl ether	2.11E-3	Inhalation	-	Inhalation	5.08E-04	-	2.14E-6
		Ingestion	-	Ingestion	5.08E-04		
Xylene	2.11E-3	Inhalation	3.69E-04	Inhalation	8.58E-03	1.56E-6	1.96E-5
		Ingestion	3.69E-04	Ingestion	7.10E-04		
Ethylbenzene	4.23E-4	Inhalation	2.36E-02	Inhalation	3.85E-04	1.01E-5	1.27E-6
		Ingestion	2.63E-04	Ingestion	2.62E-03		
Total						**9.29E-5**	**8.35E-4**

Table 5.20. LCIT method worker health results for alternative situation of metal sheet priming case

Intermediate organic chemical	**Amount (kg)**	**USEtox cancer effect factor**		**USEtox non-cancer effect factor**		**Cancer score**	**Non-cancer score**
Diesel	9.28E-4	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Isopropanol	2.11E-3	Inhalation	0	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Propylene	1.56E-3	Inhalation	0	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Benzene	1.89E-4	Inhalation	1.47E-02	Inhalation	3.72E-03	5.56E-6	1.41E-6
		Ingestion	1.47E-02	Ingestion	3.72E-03		
Toluene	2.11E-3	Inhalation	0	Inhalation	3.64E-03	7.91E-7	1.01E-5
		Ingestion	3.75E-04	Ingestion	1.14E-03		
Xylene	7.95E-4	Inhalation	3.69E-04	Inhalation	8.58E-03	5.87E-7	7.39E-6
		Ingestion	3.69E-04	Ingestion	7.10E-04		
Ethylbenzene	2.49E-4	Inhalation	2.36E-02	Inhalation	3.85E-04	5.94E-6	7.48E-7
		Ingestion	2.63E-04	Ingestion	2.62E-03		
Naphtha	3.33E-4	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Total						**1.29E-5**	**1.97E-5**

Table 5.21. Modified LCIT method results for baseline situation of metal sheet priming case

Intermediate chemical/(emission compartment)	**Amount (kg)**	**LCA ReCiPe Endpoint (E)-Human impacts (DALY)**	**LCA ReCiPe Endpoint (E)-Ecological impacts (species.yr)**
Methanol (air)	4.80E-4	1.13E-11	7.95E-15
Propylene oxide (air)	1.75E-3	7.86E-9	3.12E-13
Benzene (air)	3.20E-4	8.52E-11	4.51E-15
Chlorine (air)	1.51E-3	2.16E-7	1.02E-10
Propylene/‘propene’ (air)	1.33E-3	9.84E-11	x
Ethylene/‘ethene’ (air)	8.00E-5	5.27E-12	x
Diesel/‘petroleum distillate’ (air)	4.00E-4	x	x
Petroleum/‘petroleum oil’(air)	4.00E-4	x	x
Natural gas[1] (air)	2.10E-4	x	x
Sodium Chloride (water)	4.03E-3	x	x
Dipropylene Glycol Monomethyl Ether (air)	2.11E-3	x	x
Xylene (air)	2.11E-3	8.52E-11	2.19E-15
Ethylbenzene (air)	4.20E-4	2.23E-11	1.19E-15
Total		**2.24E-7**	**1.02E-10**

[1] Energy density of natural gas: 44.1 MJ/kg with the plant efficiency of 90% (JRC, 2017)

Table 5.22. Modified LCIT method results for alternative situation of metal sheet priming case

Intermediate chemical	**Amount (kg)**	**LCA ReCiPe Endpoint (E)-Human impacts (DALY)**	**LCA ReCiPe Endpoint (E)-Ecological impacts (species.yr)**
Isopropanol/‘2-propanol’ (air)	2.11E-3	2.62E-11	4.17E-15
Propylene (air)	1.56E-3	1.15E-10	x
Benzene (air)	1.89E-4	5.03E-11	2.66E-15
Toluene (air)	2.11E-3	2.07E-10	3.86E-15
Xylene (air)	7.95E-4	3.21E-11	8.27E-16
Ethylbenzene (air)	2.49E-4	1.32E-11	7.08E-16
Zinc (water)	9.10E-11	1.39E-14	2.16E-17
Diesel/‘petroleum distillate’ (air)	9.28E-4	x	x
Natural gas[1,2] (air)	9.28E-5	x	x
Naphtha (air)	3.33E-4	x	x
Total		**4.44E-10**	**1.23E-14**

[1] Energy density of natural gas: 44.1 MJ/kg with the plant efficiency of 90% (JRC, 2017);

[2] Natural gas standard heating value (39 MJ/m^3 (IGU, 2012)) applied to biogas

Table 5.31. LCIT method worker health results for baseline situation of PU foam production case

Intermediate organic chemical	**Amount (kg)**	**USEtox cancer effect factor**		**USEtox non-cancer effect factor**		**Cancer score**	**Non-cancer score**
Dichloromethane	6.10E-5	Inhalation	1.86E-03	Inhalation	2.17E-02	2.73E-7	2.65E-6
		Ingestion	2.62E-03	Ingestion	2.17E-02		
Methanol	1.14E-5	Inhalation	-	Inhalation	5.08E-04	-	1.16E-8
		Ingestion	-	Ingestion	5.08E-04		
Ethylene oxide	1.43E-6	Inhalation	3.20E-02	Inhalation	-	2.66E-7	-
		Ingestion	1.54E-01	Ingestion	-		
1-butanol	2.38E-6	Inhalation	-	Inhalation	2.03E-03	-	9.66E-9
		Ingestion	-	Ingestion	2.03E-03		
Ethylene	1.18E-6	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Carbon monoxide	6.49E-7	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Propylene	1.42E-6	Inhalation	0	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Total						**5.39E-7**	**2.67E-6**

Table 5.32. LCIT method worker health results for alternative situation of PU foam production case

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
Dimethyl sulfoxide	2.29E-5	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Xylene	2.58E-6	Inhalation	3.69E-04	Inhalation	8.58E-03	1.90E-9	2.40E-8
		Ingestion	3.69E-04	Ingestion	7.10E-04		
Nitrobenzene	2.04E-6	Inhalation	4.49E-02	Inhalation	2.21E-01	1.83E-7	9.02E-7
		Ingestion	4.49E-02	Ingestion	2.21E-01		
Acetone	2.04E-6	Inhalation	-	Inhalation	2.82E-04	-	1.15E-9
		Ingestion	-	Ingestion	2.82E-04		
Ethylene oxide	1.45E-6	Inhalation	3.20E-02	Inhalation	-	2.70E-7	-
		Ingestion	1.54E-01	Ingestion	-		
Phenol	9.78E-7	Inhalation	-	Inhalation	3.29E-03	-	6.44E-9
		Ingestion	-	Ingestion	3.29E-03		
Toluene	2.69E-6	Inhalation	0	Inhalation	3.64E-03	1.01E-9	1.29E-8
		Ingestion	3.75E-04	Ingestion	1.14E-03		
Methyl acetate	4.57E-5	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
1-butanol	2.63E-6	Inhalation	-	Inhalation	2.03E-03	-	1.07E-8
		Ingestion	-	Ingestion	2.03E-03		
Methanol	2.33E-5	Inhalation	-	Inhalation	5.08E-04	-	2.37E-8
		Ingestion	-	Ingestion	5.08E-04		
Propylene	8.18E-6	Inhalation	0	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Cumene	5.01E-6	Inhalation	-	Inhalation	7.69E-04	-	1.54E-8
		Ingestion	-	Ingestion	2.31E-03		
Cyclohexanol	2.04E-6	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Dichloromethane	3.05E-6	Inhalation	1.86E-03	Inhalation	2.17E-02	1.37E-8	1.32E-7
		Ingestion	2.62E-03	Ingestion	2.17E-02		

Intermediate organic chemical	**Amount (kg)**	**USEtox cancer effect factor**		**USEtox non-cancer effect factor**		**Cancer score**	**Non-cancer score**
Ethylbenzene	2.04E-6	Inhalation	2.36E-02	Inhalation	3.85E-04	4.87E-8	6.13E-9
		Ingestion	2.63E-04	Ingestion	2.62E-03		
Ethylene glycol	2.71E-6	Inhalation	-	Inhalation	6.35E-04	-	3.44E-9
		Ingestion	0	Ingestion	6.35E-04		
Isopropanol	2.01E-6	Inhalation	0	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Methyl ethyl ketone	2.10E-6	Inhalation	-	Inhalation	3.02E-05	-	1.26E-9
		Ingestion	-	Ingestion	5.68E-04		
Styrene	3.05E-6	Inhalation	4.92E-02	Inhalation	9.84E-03	1.50E-7	3.14E-8
		Ingestion	0	Ingestion	4.57E-04		
Tetrachloroethylene	2.61E-6	Inhalation	8.50E-03	Inhalation	3.23E-02	7.91E-8	1.69E-7
		Ingestion	2.18E-02	Ingestion	3.23E-02		
Benzene	8.95E-6	Inhalation	1.47E-02	Inhalation	3.72E-03	2.63E-7	6.66E-8
		Ingestion	1.47E-02	Ingestion	3.72E-03		
Total						**1.01E-6**	**1.41E-6**

Table 5.33. Modified LCIT method results for baseline situation of PU foam production case

Intermediate chemical/(emission compartment)	Amount (kg)	LCA ReCiPe Endpoint (E)-Human impacts (DALY)	LCA ReCiPe Endpoint (E)-Ecological impacts (species.yr)
Dichloromethane (air)	6.10E-5	1.13E-9	3.08E-12
Methanol (air)	1.14E-5	2.68E-13	1.89E-16
Ethylene oxide (air)	1.43E-6	1.94E-12	1.97E-16
1-butanol (air)	2.38E-6	1.79E-13	4.62E-17
Oxygen (air)	4.41E-7	x	X
Ethylene (air)	1.18E-6	7.78E-14	X
Carbon monoxide (air)	6.49E-7	1.16E-15	X
Propylene (air)	1.42E-6	1.05E-13	X
Natural gas[1,2] (air)	2.01E-6	x	X
Zinc (water)	8.55E-12	1.31E-15	2.03E-18
Total		**1.13E-9**	**3.08E-12**

[1] Energy density of natural gas: 44.1 MJ/kg with the plant efficiency of 90% (JRC, 2017);

[2] Natural gas standard heating value (39 MJ/m^3 (IGU, 2012)) applied to biogas

Table 5.34. Modified LCIT method results for alternative situation of PU foam production case

Intermediate chemical/(emission compartment)	Amount (kg)	LCA ReCiPe Endpoint (E)-Human impacts (DALY)	LCA ReCiPe Endpoint (E)-Ecological impacts (species.yr)
Methyl acetate (air)	4.57E-5	1.78E-13	3.86E-15
1-butanol (air)	2.63E-6	1.98E-13	5.11E-17
Methanol (air)	2.33E-5	5.48E-13	3.86E-16
Propylene (air)	8.18E-6	6.05E-13	X
Cumene (air)	5.01E-6	2.02E-13	1.66E-17
Cyclohexanol (air)	2.04E-6	6.96E-14	6.43E-17

Dichloromethane (air)	3.05E-6	5.66E-11	1.54E-13
Ethylbenzene (air)	2.04E-6	1.08E-13	5.80E-18
Ethylene glycol (water)	2.71E-6	1.30E-14	2.34E-18
Isopropanol (air)	2.01E-6	2.49E-14	3.97E-18
Methyl ethyl ketone (air)	2.10E-6	5.43E-14	1.22E-17
Styrene (air)	3.05E-6	2.01E-13	3.53E-18
Tetrachloroethylene (air)	2.61E-6	8.93E-11	1.04E-15
Benzene (air)	8.95E-6	2.38E-12	1.26E-16
Dimethyl sulfoxide (water)	2.83E-5	X	X
Xylene (air)	2.58E-6	1.04E-13	2.68E-18
Nitrobenzene (air)	2.04E-6	2.61E-11	3.47E-15
Acetone (air)	2.04E-6	3.91E-14	8.10E-18
Carbon monoxide (air)	1.87E-6	3.33E-15	X
Ethylene oxide (air)	1.45E-6	1.97E-12	1.99E-16
Phenol (air)	9.78E-7	4.57E-14	8.27E-16
Natural gas[1,2] (air)	5.13E-6	X	X
Toluene (air)	2.69E-6	2.64E-13	4.92E-18
Total		**7.75E-10**	**1.64E-13**

[1] Energy density of natural gas: 44.1 MJ/kg with the plant efficiency of 90% (JRC, 2017);

[2] Natural gas standard heating value (39 MJ/m^3 (IGU, 2012)) applied to biogas

Table 5.43. LCIT method worker health results for baseline situation of floor coating case

Intermediate organic chemical	**Amount (kg)**	**USEtox cancer effect factor**		**USEtox non-cancer effect factor**		**Cancer score**	**Non-cancer score**
Acetone	0.03	Inhalation	-	Inhalation	2.82E-04	-	1.66E-5
		Ingestion	-	Ingestion	2.82E-04		
Alkyl benzene sulfonate, linear	0.03	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
Ammonia	0.05	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Benzene	0.06	Inhalation	1.47E-02	Inhalation	3.72E-03	1.70E-3	4.35E-4
		Ingestion	1.47E-02	Ingestion	3.72E-03		
Benzyl alcohol	0.08	Inhalation	-	Inhalation	-	-	-
		Ingestion	0	Ingestion	-		
Benzyl chloride	0.09	Inhalation	3.32E-02	Inhalation	-	5.99E-3	-
		Ingestion	3.32E-02	Ingestion	-		
BPA epoxy-based vinyl ester resin	0.36	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
BPA powder	0.04	Inhalation	-	Inhalation	1.02E-02	-	7.32E-4
		Ingestion	-	Ingestion	1.02E-02		
Cumene	0.03	Inhalation	-	Inhalation	7.69E-04	-	9.48E-5
		Ingestion	-	Ingestion	2.31E-03		
Cyclohexane	0.02	Inhalation	-	Inhalation	8.26E-04	-	3.75E-5
		Ingestion	-	Ingestion	8.26E-04		
EDTA	0.02	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Epoxy resin	0.14	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Ethylene glycol diethyl ether	0.01	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Light fuel oil	7.46E-3	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Melamine	0.04	Inhalation	1.56E-03	Inhalation	-	1.14E-4	-
		Ingestion	1.56E-03	Ingestion	-		
Melamine formaldehyde resin	0.05	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Methacrylic acid	0.04	Inhalation	-	Inhalation	-	-	-

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
		Ingestion	-	Ingestion	-		
Phenol	0.03	Inhalation	-	Inhalation	3.29E-03	-	2.26E-4
		Ingestion	0	Ingestion	3.29E-03		
Propylene	0.05	Inhalation	0	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Propylene glycol	0.08	Inhalation	-	Inhalation	-	-	-
		Ingestion	0	Ingestion	-		
Propylene oxide	0.06	Inhalation	1.20E-02	Inhalation	2.31E-01	2.49E-3	2.81E-2
		Ingestion	2.90E-02	Ingestion	2.31E-01		
Styrene	0.15	Inhalation	4.92E-02	Inhalation	9.84E-03	7.41E-3	1.55E-3
		Ingestion	0	Ingestion	4.57E-04		
Toluene	0.07	Inhalation	0	Inhalation	3.64E-03	2.49E-5	3.17E-4
		Ingestion	3.75E-04	Ingestion	1.14E-03		
Urea, as N	0.04	Inhalation	-	Inhalation	-	-	-
		Ingestion	0	Ingestion	-		
Total						**1.77E-2**	**3.15E-2**

Table 5.44. LCIT method worker health results for alternative situation of floor coating case

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
Ammonia	0.13	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Benzene	0.07	Inhalation	1.47E-02	Inhalation	3.72E-03	2.13E-3	5.39E-4
		Ingestion	1.47E-02	Ingestion	3.72E-03		
Benzyl alcohol	0.15	Inhalation	-	Inhalation	-	-	-
		Ingestion	0	Ingestion	-		
Benzyl chloride	0.18	Inhalation	3.32E-02	Inhalation	-	1.21E-2	-
		Ingestion	3.32E-02	Ingestion	-		
	0.64	Inhalation	x	Inhalation	x	x	x

Intermediate organic chemical	Amount (kg)	USEtox cancer effect factor		USEtox non-cancer effect factor		Cancer score	Non-cancer score
BPA epoxy-based vinyl ester		Ingestion	x	Ingestion	x		
BPA powder	0.03	Inhalation	-	Inhalation	1.02E-02	-	6.16E-4
		Ingestion	-	Ingestion	1.02E-02		
EDTA	0.13	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Epoxy resin	0.25	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Light fuel oil	0.03	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Melamine	0.04	Inhalation	1.56E-03	Inhalation	-	1.22E-4	-
		Ingestion	1.56E-03	Ingestion	-		
Melamine formaldehyde resin	0.05	Inhalation	x	Inhalation	x	x	x
		Ingestion	x	Ingestion	x		
Meta-phenylene diamine	0.04	Inhalation	-	Inhalation	4.24E-02	-	3.61E-3
		Ingestion	0	Ingestion	4.24E-02		
Methacrylic acid	0.08	Inhalation	-	Inhalation	-	-	-
		Ingestion	-	Ingestion	-		
Phenol	0.03	Inhalation	-	Inhalation	3.29E-03	-	1.91E-4
		Ingestion	0	Ingestion	3.29E-03		
Styrene	0.27	Inhalation	4.92E-02	Inhalation	9.84E-03	1.33E-2	2.78E-3
		Ingestion	0	Ingestion	4.57E-04		
Toluene	0.14	Inhalation	0	Inhalation	3.64E-03	5.14E-5	6.55E-4
		Ingestion	3.75E-04	Ingestion	1.14E-03		
Urea, as N	0.07	Inhalation	-	Inhalation	-	-	-
		Ingestion	0	Ingestion	-		
Total						**2.77E-2**	**8.39E-3**

Table 5.45. Modified LCIT method results for baseline situation of floor coating case

Intermediate chemical/(emission compartment)	Amount (kg)	LCA ReCiPe Endpoint (E)-Human impacts (DALY)	LCA ReCiPe Endpoint (E)-Ecological impacts (species.yr)
Acetone (air)	0.03	3.24E-09	1.35E-13
Alkyl benzene sulfonate, linear (water)	0.03	-	1.74E-10
Ammonia (air)	0.05	4.14E-06	2.05E-09
Benzene (air)	0.06	5.63E-08	8.53E-13
Benzyl alcohol (air)	0.08	-	9.02E-11
Benzyl chloride (air)	0.09	2.56E-07	2.03E-11
BPA epoxy-based vinyl ester resin (water)	0.36	-	-
BPA powder (water)	0.036	3.81E-08	4.85E-10
Chlorine (air)	0.10	1.42E-05	6.53E-09
Cumene (air)	0.03	3.34E-09	1.15E-13
Cyclohexane (air)	0.02	2.21E-09	6.92E-14
EDTA (water)	0.02	-	6.03E-13
Epoxy resin (water)	0.14	-	-
Ethylene glycol diethyl ether (air)	0.01	-	-
Hydrogen cyanide (air)	0.02	1.68E-06	1.14E-08
Light fuel oil (air)	7.46E-3	-	-
Melamine (water)	0.04	1.62E-09	2.81E-12
Melamine formaldehyde resin (water)	0.05	-	-
Methacrylic acid (air)	0.04	-	1.75E-10
Phenol (air)	0.03	2.22E-08	3.81E-11
Propylene (air)	0.05	3.57E-09	-
Propylene glycol (air)	0.08	2.28E-09	3.15E-11
Propylene oxide (air)	0.06	1.81E-06	1.21E-11
Styrene (air)	0.15	3.34E-07	2.61E-13
Toluene (air)	0.07	4.08E-08	1.36E-13
Urea, as N (water)	0.04	-	2.03E-13
Total		**2.26E-05**	**2.10E-08**

Table 5.46. Modified LCIT method results for alternative situation of floor coating case

Intermediate chemical/(emission compartment)	**Amount (kg)**	**LCA ReCiPe Endpoint (E)-Human impacts (DALY)**	**LCA ReCiPe Endpoint (E)-Ecological impacts (species.yr)**
Ammonia (air)	0.13	1.09E-05	5.38E-09
Benzene (air)	0.07	6.98E-08	1.06E-12
Benzyl alcohol (air)	0.15	-	1.82E-10
Benzyl chloride (air)	0.18	5.18E-07	4.09E-11
BPA epoxy-based vinyl ester (water)	0.64	-	-
BPA powder (water)	0.03	3.20E-08	4.08E-10
EDTA (water)	0.13	-	5.10E-12
Epoxy resin (water)	0.25	-	-
Hydrogen cyanide (air)	0.07	5.06E-06	3.43E-08
Light fuel oil (air)	0.03	-	-
Melamine (water)	0.04	1.74E-09	3.02E-12
Melamine formaldehyde resin (water)	0.05	-	-
Meta-phenylene diamine (water)	0.04	1.55E-08	-
Methacrylic acid (air)	0.08	-	3.15E-10
Phenol (air)	0.03	1.89E-08	3.24E-11
Sodium cyanide (water)	0.07	-	-
Styrene (air)	0.27	6.00E-07	4.67E-13
Toluene (air)	0.14	8.44E-08	2.82E-13
Urea, as N (water)	0.07	-	3.25E-13
Total		**1.73E-05**	**4.07E-08**

‘Thinner 1’

Calculation of energy required to vaporize the thinner

Table 5.57. Evaporation energy of constituent chemicals of ‘Thinner 1’

CAS No.	**Name**	**Evaporation energy (kJ/kg)**
107-98-2	1-methoxy-2-propanol	362
1330-20-7	Xylene	409
100-41-4	Ethylbenzene	398
1589-47-5	2-methoxypropanol	-

By using Fig. 5.4 and Table 5.57:

Heat energy needed to vaporize ‘Thinner 1’ = (1474 kg*362 kJ/kg+1474 kg*409 kJ/kg+295 kg*398 kJ/kg)/1000 = 1,254 MJ

Amount of transport

Lorry, 7.5–16 metric tons, EURO3 (RER) was selected as the type of transport. The total amount of chemicals in Table 5.57 is equal to 3,248 kg. This amount when transported over 1,700 km (from Germany to Lithuania) is equivalent to 5,522 tkm.

‘Thinner 2’

Calculation of energy required to vaporize the thinner

Table 5.58. Evaporation energy of constituent chemicals of ‘Thinner 2’

CAS No.	Name	Evaporation energy (kJ/kg)
67-63-0	Isopropanol	779
108-88-3	Toluene	351
1330-20-7	Xylene	409
100-41-4	Ethylbenzene	398
64742-95-6	Solvent Naphtha	1110

By using Fig. 5.5 and Table 5.58:

Heat energy needed to vaporize ‘Thinner 2’ = (1474 kg*779 kJ/kg+1474 kg*351 kJ/kg+555 kg*409 kJ/kg+174 kg*398 kJ/kg+208 kg*1110 kJ/kg)/1000 = 2,193 MJ

Amount of transport

Lorry, 7.5–16 metric tons, EURO3 (RER) was selected as the type of transport. The total amount of chemicals in Table 5.58 is equal to 3,885 kg. This amount when transported over 1,700 km (from Germany to Lithuania) is equivalent to 6,605 tkm.

Annex III

The sum of two or more normal distributions:

Let us assume two life cycle processes (parallel or series) with emission distributions of $P(x) = \frac{e^{-(x-\mu)^2/2\alpha^2}}{\alpha\sqrt{2\pi}}$ and $P(y) = \frac{e^{-(y-\gamma)^2/2\beta^2}}{\beta\sqrt{2\pi}}$; here, x and y are the amounts of each emission, μ and γ are the means, and α and β are the standard deviations (σ_s) of each distribution. The sum is given by $P(z) = \iint_{-\infty}^{\infty} P(x)P(y)dxdy$, where z = x + y. If we assume that z is constant and solve P(z), we get $\mathrm{P(z)} = \frac{\alpha\beta e^{-\alpha^2\beta^2(z-\mu-\gamma)^2/2(\alpha^2+\beta^2)}}{\sqrt{2\pi(\alpha^2+\beta^2)}}$. Hence, $\alpha^2 + \beta^2 = \sigma_z{}^2$, where σ_z is the standard deviation P(z). If we assume that $\alpha = \beta = \sigma_s$, then we can write $\sqrt{2}\sigma_s = \sigma_z$. P(z) can be summed up further with another normal distribution in the same way, and, for the sum of n distributions, the resultant distribution has the standard deviation of $\sqrt{n}\sigma_s = \sigma_z$. Hence the standard deviation per process is given by $\sigma = {\sigma_s}/{\sqrt{n}}$.

This result indicates that as we increase the number of life cycle processes, regardless of being parallel or series to each other, the random errors per process decrease; and, given enough processes and considering only random mistakes, inexpert and expert assessors obtain very close results (and, for an infinite amount of processes, they get the same result).

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Išleido Kauno technologijos universitetas, K. Donelaičio g. 73, 44249 Kaunas
Spausdino leidyklos „Technologija“ spaustuvė, Studentų g. 54, 51424 Kaunas