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Corporate Textile Chemical Management

How to Avoid Problem Shifting

Master's thesis in Master Programme
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Abstract

In the drive towards both a circular economy and a non-toxic environment, a major challenge is hazardous chemicals in products. Textile production involves the use of many different chemicals and its value chain is often very complex, which complicates the management of chemicals throughout this supply chain.

In this master thesis, a life cycle assessment (LCA) and risk assessment (RA) were carried out in a case study on two chemicals (chemical A and B) produced by AkzoNobel, used to produce industrial textile softeners. Due to concern about reproductive toxicity regarding chemical A, there is a growing interest in softener produced using other chemicals (such as chemical B). However, as the softener produced using chemical B requires higher temperature when used, there is a risk of problem shifting in this chemical substitution case.

The thesis also covered possible ways to integrate the two tools (RA and LCA), which can be done on methodological level or by combining the results. In the case study, this was done by carrying out the RA throughout the life cycle, while also including toxicity impact of chemical A and B in the LCA done on the softeners. The LCA result was then aggregated into disability-adjusted life years (DALY) to express the burden on human health. Aggregating results is a way to make the result more comprehensive and easier to communicate.

In this RA, there were no uncontrolled risks. While the exposure to consumers was very low, the calculated exposures to workers were for some activities almost high enough for risk of adverse effects to occur. There were however significant uncertainties involved in the exposure to workers. The LCA showed that softener based on chemical B had only a slightly higher impact (for the studied impact categories and resulting DALYs) than softener based on chemical A. However, only using softener based on chemical B, and instead incinerating chemical A, would result in a higher impact than the current use of both types of softener. Utilising the generated heat from this incineration for energy recovery did not significantly decrease this impact. The result of this case study indicates that problem shifting could occur if switching from chemical A to chemical B based softener.

Key words: circular economy, non-toxic environment, risk assessment, life cycle assessment, disability-adjusted life years, textile softener

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Abbreviations

A-LCA - Attributional Life Cycle Assessment

BMD - Benchmark Dose

BMDL - Benchmark Dose Lower Confidence Limit

C2C - Cradle to Cradle

CF - Characterisation Factor

CIP - Chemicals in Products

C-LCA - Consequential Life Cycle Assessment

CLP - Classification, Labelling and Packaging

CMM - Chemical Management Module

CMR - Carcinogenic, Mutagenic or toxic to Reproduction

CSA - Chemical Safety Assessment

CSR - Chemical Safety Report

CTU - Comparative Toxic Units

DALY - Disability-Adjusted Life Years

DNEL - Derived No Effect Level

DOC - Dissolved Organic Carbon

EAP - Environmental Action Programme

ECETOC TRA - European Centre for Ecotoxicology and Toxicology of Chemicals Targeted Risk Assessment

ECHA - European Chemicals Agency

ED50 - Effective Dose 50 (where 50% of the population show the effect)

EF - Emission Factor

EPS - Eco Premium Solutions

ERC - Environmental Release Category

EU - European Union

FU - Functional Unit

GHS - Globally Harmonized System of Classification and Labelling of Chemicals

GOTS - Global Organic Textile Standard

GPP - Green Public Procurement

LCA - Life Cycle Assessment

LCBRA - Life Cycle Based Risk Assessment

LCI - Life Cycle Inventory Analysis

LCIA - Life Cycle Impact Assessment

LOAEL - Lowest Observed Adverse Effect Level

MCDA - Multi-Criteria Decision Analysis

NOAEL - No Observed Adverse Effect Level

OECD - Organisation for Economic and Cooperation and Development

PBT - Persistent, Bioaccumulative and Toxic

PDF - Potentially Disappeared Fraction of Species

PNEC - Predicted No Effect Concentration

PROC - Process Category

RA - Risk Assessment

RCR - Risk Characterisation Ratio

REACH - Registration, Evaluation, Authorisation and Restriction of Chemicals

RSL - Restricted Substance List

STP - Sewage Treatment Plant

SVHC - Substance of Very High Concern

TOC - Total Organic Carbon

vPvB - very Persistent and very Bioaccumulative

WSSD - World Summit of Sustainable Development

WWTP - Wastewater Treatment Plant

ZDHC - Zero Discharge of Hazardous Chemicals

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1. Introduction

The chemically intensive textile industry contributes to many environmental problems, for example with its high use of water and energy (Börjeson, 2017). The textile industry also involves the use of chemicals that have been shown to be hazardous, and some of these have even been found in human blood and deep in the ocean (Börjeson, 2017). The trend of fast fashion (see for example, Joy et al., 2012) increases the consumption of textiles, and makes chemical management within the textile industry even harder to handle, as it can make it difficult to predict what chemicals will be used and for what purpose.

While the textile industry has previously often prioritised things like the functionality and price for the garment, social sustainability and climate change (Börjeson, 2017), there has also been an increasing interest in managing chemical risks related to the chemicals in textile products. This is in line with increasing efforts in society to decrease the exposure to hazardous chemicals, as evident by Sweden's Non-Toxic Environment quality objective (Swedish Environmental Protection Agency, 2016) and efforts being made on the EU level such as the 7th Environmental Action Programme, that involves the development of a strategy for non-toxic environment as well as a transition to a circular economy (European Commission, 2017c).

This master thesis explored how corporate textile management strategies can take both the non-toxic environment and circular economy principles into consideration. The focus was a case where chemical risks and other potential environmental impacts of two chemicals produced by AkzoNobel were analysed. *Chemical A* and *chemical B* can be used as intermediate chemicals in softener production. Whereas chemical A is typically the most preferred of the two in terms of performance (AkzoNobel, 2018, personal communication), studies have shown toxicity to reproduction (ECHA, n.d.-b). Due to this concern, there is an increasing interest in chemical A free softener, where chemical B is a possible alternative (AkzoNobel, 2018, personal communication). However, a concern regarding chemical B is that its use in softener would generate higher environmental impact in other impact categories. Replacing chemical A with chemical B could hence lead to shifting of burden between impact categories.

1.1 Aim

The aim of this master thesis was to address the risk of problem shifting in this chemical substitution case, by conducting a life cycle assessment (LCA) and a risk assessment (RA) for chemical A and chemical B. The aim was furthermore to investigate the opportunities to create a combined product safety and life cycle assessment based tool for AkzoNobel's chemicals management, guided by the principles of non-toxic environment and circular economy.

1.2 Objectives

The thesis work can essentially be divided into three main objectives:

- Define "toxic free environment" in terms of guiding principles and tools for corporate chemicals management, and identify the implications of these principles in a circular economy framework. This included a literature review mapping how the chemical legislation process works (with focus on the textile sector); describing current and foreseen chemical regulation; the political/policy landscape affecting the regulatory development; and relevant industry initiatives for chemicals management.
- Develop a framework for a combined product safety and life cycle based assessment tool. This was done through a case study, in which an LCA and an RA was performed on two chemicals, and their end use application as an industrial fabric softener. The goal with the LCA was to analyse the difference in environmental impacts between the current softener manufacture and use, and a future scenario with a discontinued use of chemical A. The goal with the RA was to analyse if there is a risk of unacceptable adverse effects from using any of the two softeners. The possibilities to combine the assessment methods, or their results, in a new framework was explored starting from a literature review of published reports on attempts to such combinations.
- Propose how the results can be made communicable to policy makers.

1.3 Thesis Outline

The report begins with a background chapter, based on the literature study made on "toxic free environment", circular economy and current regulations with focus on the textile industry. This chapter also includes the literature review on possible ways to combine LCA and RA. Then a method chapter follows, which covers the basis for the RA and LCA, as well as a technical description of the system in question. Thereafter the results from these tools are presented, together with a recommendation on how results like this can be compared and combined. Lastly, a discussion follows, leading up to a conclusion chapter and recommendations for future studies. The thesis report also includes appendix containing more detailed graphs and tables of the results.

This thesis is the public report of the Master thesis project. Complementary to this report are a number of confidential appendices.

1.4 Limitations

- The literature review on policy mapping was limited to focus on chemical management related to the textile industry supply chain.
- The LCA was limited to include environmental potential impacts and does not include social potential impacts. Both the LCA and the RA were limited to cover normal operations while potential impacts in case of accidents was not assessed.
- Due to confidentiality surrounding the two chemicals in question, information that could reveal the chemical identities had to be excluded from this report. This also applies for some of the process information, for example the amount and type of raw materials used.
- The third objective was limited to a discussion.

The opinions presented in this master thesis are our own, and do not necessarily represent the views of the AkzoNobel company. The intended audiences of this case study are mainly AkzoNobel as the producer, the softener producer as the customer of AkzoNobel and the general public. It is important to note that while the European Chemicals Agency (ECHA) guidance on chemical safety assessment (CSA) and ISO standards on LCA was used as guidance to conduct the RA and LCA, these were only used as guidance and were not strictly followed. Hence, this is for example, not an ISO-LCA as such.

2. Background

"*In 2050, we live well, within the planet's ecological limits. Our prosperity and healthy environment stem from an innovative, circular economy where nothing is wasted and where natural resources are managed sustainably, and biodiversity is protected, valued and restored in ways that enhance our society's resilience. Our low-carbon growth has long been decoupled from resource use, setting the pace for a safe and sustainable global society.*" - European Commission (2016)

This is a vision by the European Union (EU), and to guide us towards this goal, the 7th European Environmental Action Programme (EAP) is currently used (European Commission, 2016).

2.1 A Non-Toxic Environment

One of the objectives in the 7th EAP is to protect from risks to human health and the environment, for which a strategy for non-toxic environment is being formed (European Commission, 2017c). A non-toxic environment is also one of the environmental quality objectives that Sweden has set up to reach the generational goal, that should be fulfilled by 2020: *"The overall goal of environmental policy is to hand over the next generation a society in which the major environmental problems have been solved, without increasing environmental and health problems outside Sweden's borders."* - Swedish Environmental Protection Agency (2016, pp 3)

In total, the Swedish Parliament has adopted 16 environmental quality objectives. *A Non-Toxic Environment*, which is the area of focus in this thesis, is defined as: *"The occurrence of man-made or extracted substances in the environment must not represent a threat to human health or biological diversity. Concentrations of non-naturally occurring substances will be close to zero and their impacts on human health and on ecosystems will be negligible. Concentrations of naturally occurring substances will be close to background levels."* - Swedish Environmental Protection Agency (2016, pp 12). The goal of this objective is hence to achieve sustainable production and use of chemicals, for safer products, articles and services (Swedish Chemicals Agency, 2015a). Different government agencies are connected to different quality objectives and have certain responsibilities in helping to achieve them, guided by the Swedish Environmental Protection Agency (Swedish Environmental Protection Agency, 2016). The Swedish Chemicals Agency is the responsible authority for 'a non-toxic environment' (Swedish Chemicals Agency, 2015a).

There are a number of milestone targets connected to the environmental quality objectives that are used to indicate the steps needed to achieve the environmental quality objectives and the environmental goal (Swedish Environmental Protection Agency, 2017). The milestone targets are divided into five areas. The area connected to the non-toxic environment objective is *dangerous substances*, which includes the following subjects (Swedish Environmental Protection Agency, 2017):

- Particularly dangerous substances
- Knowledge on the health and environmental properties of substances
- Information about dangerous substances in articles
- Development and application of the EU's chemical rules
- More effective chemicals supervision in the EU
- Non-toxic and resource-efficient ecocycles
- Reducing children's exposure to dangerous chemicals
- Greater environmental consideration in the EU pharmaceuticals legislation and internationally

These subjects then include the different milestone targets. An example of one of the milestone target underneath *Particularly dangerous substances* is: "*By 2018, particularly dangerous substances are subject to examination or phase-out decisions under current regulations in all areas of use.*" - Swedish Environmental Protection Agency, (2017)

One may then wonder what exactly is a "particularly dangerous substance"? The Swedish Chemicals Agency have made the web-based PRIO tool, in which the selection of substances to phase-out is based on the Swedish non-toxic environment environmental objective and reflect criteria in the REACH regulation (Swedish Chemicals Agency, 2016a). The criteria for "particularly hazardous substances" is: substances that are Carcinogenic, Mutagenic or toxic to Reproduction (CMR) category 1A (known to cause the effect) and 1B (suspected to cause the effect), endocrine disruptors, particularly hazardous metals (Hg, Pb, Cd) and Persistent, Bioaccumulative and Toxic (PBT) or very Persistent and very Bioaccumulative (vPvB) substances (Swedish Chemicals Agency, 2016a; ChemSafetyPro, 2017). Substances that are toxic to reproduction are "*Substances that by inhalation, swallowing or uptake through the skin can cause, or increase the incidence of, non-heritable damage to the offspring or impaired male or female fertility. "*- Swedish Chemicals Agency (2015b).

Progress towards each of the environmental quality objectives is reviewed annually in a follow-up report, and every four years a more in-depth evaluation is made (Swedish Environmental Protection Agency, 2016). The reported progress towards the objectives forms the basis of the Swedish Government's policy and priorities. For example, the Parliament can decide on different taxes and laws to further increase the effort. In order to assess the progress, different indicators are used (Swedish Environmental Protection Agency, 2018a). In order to achieve the environmental goals in Sweden by 2020, several actors need to cooperate (Swedish Environmental Protection Agency, 2016). Efforts at local and regional levels, for example in the municipalities, but also action at the EU level, for example to reduce harmful emissions, are needed. The business community plays a crucial role through their efforts as well. Thanks to action on the political level, such as environmental laws, stricter legislation and international agreements, as well as voluntary measures, there has in fact been a decreased use of many hazardous substances in recent decades. However, there are still many challenges left to overcome, for example, a big gap between the number of chemicals used compared to those that have been evaluated for hazardous properties or regulated (European Commission, 2017a).

In a recent follow up on all the environmental quality objectives, it was reported that despite all the measures taken by the Swedish Government and the authorities, the objectives will not be

achieved by 2020 (Swedish Environmental Protection Agency, 2018b). Only two out of the 16 objectives have been or may be reached by 2020; non-toxic environment is not one of them. Measures taken trying to reach the non-toxic environment have mainly focused on limiting the exposure to children, for example regarding hazardous chemicals in toys and electronics. The Swedish Environmental Protection Agency (2016) believes more international agreements and technological developments are needed, as well as a better understanding on the hazardous properties of chemicals and possible restrictions of their use.

2.2 Circular Economy

In short, circular economy is the shift away from linear flows and instead creating closed loops. Geissdoerfer et al. (2017, pp 759) defines circular economy as: "*A regenerative system in which resource input and waste, emission, and energy leakage are minimised by slowing, closing, and narrowing material and energy loops. This can be achieved through long-lasting design, maintenance, repair, reuse, remanufacturing, refurbishing, and recycling*".

Comparing the concept of sustainability with the one of circular economy, Geissdoerfer et al. (2017) highlights the difference in responsibilities. The circular economy framework evolves around measures taken by private business, regulators and policymakers - whereas the responsibilities in terms of sustainability are shared by everyone. According to Geissdoerfer et al. (2017), who did a literature study and analysis on these concepts, many view a circular economy as one of the possible ways towards sustainability, but not necessarily a necessity. While circular economy is believed by many to have a positive impact on some sustainability aspects, such as resource efficiency and job creation, it is not always viewed as a sufficient condition towards sustainability. For example, according to Geissdoerfer et al. (2017), some claim circular economy does not help with other aspects of sustainability, like the social dimension. Completely circular flows might not be possible in combination of increased demand for different products and materials. It might also be the case that recycling materials requires more energy than acquiring virgin material, meaning a circular flow could cause higher environmental impact in terms of greenhouse gas emissions. Hazardous substances are another concern for the circular economy framework as the reuse and recycling of materials can recirculate hazardous chemicals as well. ChemSec (2016) argues that hazardous substances should be kept out of these closed loops, and phased out from virgin and recycled material. Because if materials containing hazardous substances would be reused or recycled, this would not mean a sustainable and safe circular economy.

2.3 Textile Industry Value Chain

Globalisation has affected the supply chains of many industries, and as a result the supply chain of different industries have become more complex (Börjeson, 2017). This has made it harder to govern environmental and health problems. One example is the textile industry, whose global supply chain makes it hard to manage this chemically intensive business. Different steps in the textile industry's supply chain can be located in many different countries, which according to Börjeson (2017) can complicate for example, complying with regulations, as communications throughout the supply chain can be lacking and it can be unclear who is responsible for what. Through successful management of supply chains, companies can achieve a comparative

advantage. But according to Börjeson (2017), there are several challenges for those striving for what she calls responsible supply chain management, such as uncertainty regarding chemical risks. During her study about responsibility of risks connected to toxic chemicals in the textile value chain, Börjeson (2017) could see an increasing pressure on actors to take responsibility, she also noticed that more and more actors in the textile industry showed a bigger commitment in managing chemical risks. For example, voluntary tools become more popular, such as labels, codes of conduct and using restricted substances lists.

Textile production processes involves several main steps; from fibre production (including cultivation in the case of natural fibres), yarn spinning, knitting, wet treatment and final product making process as figure 2.1 (Roos, 2015a). Based on a report by Roos (2016), the adverse effect related to chemicals in textile life cycle is mainly found in connection to the wet treatment. The use of detergents, lubricants, softeners, bleach, dye stuff and finishing agents contribute to several impacts such as acidification, eutrophication, ecotoxicity and human toxicity.

Figure 2.1 General process of textile production (of a knitted product).

A study on 3500 chemicals that can be used in textile production found that 10% of these were identified as particularly hazardous (Swedish Chemicals Agency, 2016b). However, this was believed to be an underestimation. Furthermore, textile production outside of the EU stands for 80% of the textile products on the EU market. These are not covered by REACH regulation to the same extent as those products produced within EU, resulting in information gaps.

2.4 Current Legislation and Voluntary Actions to Manage Chemical Risks

In Europe, two of the main chemical regulations are REACH and the Classification, Labelling and Packaging (CLP) Regulation (European Commission, 2017a). These regulations, that are related to the production and use of chemicals, has been established to prevent environmental and health risks along the life cycle of the chemical substance. REACH is a regulation by the European Union mainly directed towards companies (ECHA, n.d.-a). It stands for Registration, Evaluation, Authorisation and Restriction of Chemicals, and requires companies to share information on the substances they handle. Chemicals used in textile manufacturing are covered by the regulation, but unless a chemical is identified as a Substance of Very High Concern (SVHC) or is covered by a restriction, chemicals in imported textiles are not covered (Retail Forum, 2013). Regarding restrictions of CMR substances, a restriction of CMRs 1A and 1B in textiles might be on the way (European Commission, 2018). There are also regulations related to specific sorts of products, such as the Toys Directive and the Medical Devices Directive. Europe's regulation also has a target to increase communication between the chemical industry and the downstream manufacturers, which will support the work of reaching the chemical management target 2020 which was set in the World Summit of Sustainable Development in Johannesburg (WSSD) (European Commission, 2017a). The target is to ensure chemicals will be managed with life cycle perspective in order to minimize the risks on human and environment

(European Commission, 2013). A regulation at international level is the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) which sets a standard to classify and label the chemical based on the hazard criterion (United Nations, 2005).

Beside setting requirements on the analysis of chemicals in textile products, most of the regulations in the EU related to clothing manufacturing also set rules for imports from low-income countries (Retail Forum, 2013). This is necessary since chemical legislations and requirements in Europe are stricter than in other countries. For instance, Zhang (2009) who did a master thesis on textile supply chain in China, found that regulation related to textile chemicals in China set a lower standard compared with what has been applied in Europe. Some chemicals that are restricted to use in Europe's textile manufacturing industry are still allowed to be used in China. It is also important to note that the databases on hazardous substances are more often updated in Europe than those in China. China has agreed to follow international conventions about chemical use (Zhang, 2009). China also have regulations on their own, where pollution of water bodies from the textile industry is given high priority.

The global production and use of chemical substances are increasing and, according to the European Commission (2017a), in 2014 the sales of chemical products on the global market was twice as high as 10 years before. The vast number of chemical products make chemical management difficult, especially in complex and global supply chains. To support the chemical management the United Nations has conducted the Chemicals in Products (CIP) programme that aims to make it easier for companies and stakeholders to share information about the chemicals contained in their products. Based on this program and the exchange information system, the manufacturing sectors which use chemical substances in their production processes are able to choose the chemicals based on hazard characteristics and the information provided with different references (UNEP, 2015). There are also organisations that have chemicals lists based on specific effects that can be used by the industry to phase-out hazardous chemicals. For example, State of California Environmental Protection Agency has a chemicals list for cancer and reproductive effects (UNEP, 2015). One of the main voluntary instruments related to chemical industry and downstream process is EU Green Public Procurement (GPP) criteria which group chemicals based on the final concentration on the textile products (European Commission, 2017b). It also includes the test methods and the products' information disclosure which is called Restricted Substance Lists (RSLs). Specific to textile products, there are also several different voluntary actions that have been established by different stakeholders. For example, major clothing companies have joined together in the Zero Discharge of Hazardous Chemicals (ZDHC) Programme, to make a list of chemicals that they believe should be banned in the production of their products (ZDHC Foundation, 2015). Ecolabels are a form of voluntary actions and can be used by the textile industry to communicate to the consumers that their products fulfil certain sustainability criteria set by the ecolabel (Roos, 2016). It is also helpful for the companies to improve their production process. There are several types of ecolabels that can be applied within the textile business. Currently, 107 ecolabels exist in the Ecolabel Index for textile products (Ecolabel Index, 2016). The three most common environmental ecolabels are OEKO-TEX, bluesign, and Global Organic Textile Standard (GOTS), which are described further below. While OEKO-TEX is mainly to prevent toxic chemicals in the products, bluesign and GOTS are more focused on chemicals management along the whole textile supply chain (Roos, 2016).

- The OEKO-TEX label certifies that the textile products have been tested. The tests are focused on the release of hazardous substances from the garment and skin contact, but depending on the type of material and target group, additional testing on colour fastness and emissions to air can also be performed (OEKO-TEX® Association, n.d.). If the materials have atypical odours this will affect the certification as well. There are certain criteria regarding the testing procedures for how these tests should be performed (OEKO-TEX® Association, 2018)
- The bluesign labelling system aims to eliminate harmful chemicals in the textile production and setting the standards for environmental friendly and safe manufacturing process. Its main purpose is to ensure that the final products from textile industry fulfil the safety requirements for the customers (bluesign® technologies ag, n.d.). The usage ban in the bluesign system aims to prevent the presence of substances in the textile production and prevent the harmful emission to environment (bluesign® technologies ag, 2017). It means that the chemicals with usage ban is prohibited in the textile product manufacturing if a product is to fulfil the bluesign criteria. Besides bans on chemicals use bluesign also have limit values, defined as "*The maximum amount of chemical substances permitted in articles for the usage ranges A, B and C*" (bluesign® technologies ag, 2017, pp 4). These are the different usage ranges:
    - A: Close to skin use and baby-safety with age 0-3 years
    - B: Occasional skin contact
    - C: No skin contact

2.5 Assessment Tools in Textile Industry

There are several assessment tools available to be used in textile chemicals management for safety and sustainability. RA can be used to assess if there are any unacceptable risks to human health or the environment for chemicals used in the textile industry. Other tools can be used to assess sustainability in a broader sense, including more than chemical risks in the textile company, such as LCA, Cradle to Cradle (C2C), and the Higg Index (Roos, 2016). These tools are essential in developing new technologies, particularly to prevent the risk of shifting the environmental consequences from one phase to another in the life cycle of textile products. It can also be used to ensure that the new technology will not create problem shifting between different types of environmental impacts. For the evaluation of management routines, Higg Index and its Chemical Management Module (CMM) are commonly used. However, Higg Index and C2C are not applicable to assess the impact and compare textile technologies in a quantitative way like LCA.

The two tools that were used for the case study in this thesis is LCA and RA (chemical safety assessment). These methods are further explained in the following sections.

2.5.1 Risk Assessment

In chemical management it is important to distinguish between hazard and risk. To put it simply, risk can be seen as the probability of a hazard resulting in actual damage (Kaplan and Garrick, 1981). In other words, while a chemical substance can have inherent hazardous properties, it does not necessarily mean that someone will be exposed and harmed.

To assess chemical risks in different contexts guidelines have been developed. The EU REACH CSA guidance is commonly used to assess chemicals in terms of intrinsic hazardous properties and using exposure scenarios, to see if the risks are controlled or not (ECHA, 2011). In a step called "hazard assessment", information about the toxicity of the chemicals are collected. This includes what type of adverse effects that can be caused by the chemicals and at which levels no adverse effects are expected (so called no effect levels). The possible level of exposures are then calculated in the "exposure assessment". These two steps then meet in the "risk characterisation", in which the exposure levels are compared to the no effect levels. If the exposure is equal to or higher than the no effect level, there is an uncontrolled risk - as exposure higher than the no effect level can result in adverse effects.

2.5.1.1 Chemical Properties

One of the main inputs to a chemical RA is of course a description of the properties if the chemical(s) in question. Standardized testing protocols aim at assuring high quality and comparability between studies. The Organisation for Economic and Cooperation and Development (OECD) has developed a number of guidelines to test chemicals for physico-chemical properties, effects on biotic systems, environmental fate and behaviour and health effects and those are frequently used in chemical RA, especially in regulatory contexts. Two types of tests, particularly relevant in this case, are further described below.

For toxicity to reproduction, there are a number of different tests (OECD, n.d.). For example, the OECD guidelines 421 and 422 for the testing of chemicals are two reproductive toxicity screening studies. They can be used to see effects on reproductive performance caused by the substances (ECHA, 2012). However, as these screening tests only provide limited information about the effects and have lower sensitivity, reproductive toxicity studies like OECD test guidance 414 and 416 are also needed. OECD test guidance on identification on reproductive toxicity (for example, 414 and 416) can be used to determine whether or not a substance is toxic to reproduction and can be used as a more certain basis to derive no effect levels.

The OECD also has testing guidelines for analysing if chemical substances are biodegradable (OECD, 1992). That a substance is biodegradable means that it can be broken down by microbial activity (Swedish Chemicals Agency, 2015c). Tests 301 can be used to assess the biodegradability of chemicals in aerobic aqueous medium (OECD, 1992). There are different requirements that the substance needs to meet to be considered biodegradable. For example, to be ready biodegradable a removal of dissolved organic carbon (DOC) needs to reach 70%, within 10 days of the usually 28 days long tests according to the OECD 301 standard.

2.5.2 Life Cycle Assessment

LCA is method for assessing the flows and environmental impacts of systems and can be used by companies to improve their environmental performance (Baumann and Tillman, 2004). In LCA, the first step is to make a goal and scope definition regarding the product or system for which the environmental impact should be assessed, and thereafter do a life cycle inventory analysis (LCI). In this step, input data, like raw materials and energy, and output data, like products, waste and emissions, are collected for each process, and linked to a functional unit. The functional unit describes the function of the analysed product or system. In the next step of LCA, which is life cycle impact assessment (LCIA), these emissions are then "translated" (using characterisation

factors (CFs)) into different kinds of environmental impacts. The potential impacts can be assessed in midpoint or endpoint level, or can be performed at both points. While midpoint represents different environmental impacts, in the form of different impact categories, such as global warming potential (climate change potential), eutrophication potential, etc.; in the endpoint level, these impacts are aggregated into the effect that can be seen on human health, ecosystem, and resources.

In the the ILCD Handbook on LCIA, there are several impact categories in the midpoint level (European Commission, 2011), with several characterisation methods recommended by ILCD to calculate the environmental impacts (European Commission, 2012). For climate change, IPCC 2007 method is recommended. However, there are some emissions that are not in the IPCC's list then taken from ReCiPe2008 method. For ILCD recommended CFs, the CFs for ozone depletion was determined from ReCiPe2008 and Meteorological Organisation WMO (1999), while USEtox is the recommended method for toxicity impact.

There are two main types of LCA: attributional (A-LCA) and consequential (C-LCA). A-LCA analyse environmental impacts based on all the input and output flows in the life cycle (Ekvall and Weidema, 2004). The starting point for LCA is the specific functional unit, so the A-LCA analysis will include all the emission connected to it. The C-LCA mainly focuses on assessing the impacts when there is a change in the system that is investigated. It describes all the relevant flows that are affected by this change, including the system outside the life cycle (also with functional unit as starting point).

LCA can be used to assess possible substitution of hazardous chemicals. Since LCA can be quite time intensive, many frameworks have instead used life cycle thinking. Jacobs et al. (2016) found that a big challenge for alternative assessments is the lack of data, regarding the exposure to hazardous chemicals as well as their inherent hazardous properties. Jacobs et al. (2016) concluded that methods to quickly evaluate possible exposure are needed, as these types of assessments need to be rather quick and flexible in order for smaller firms to have the resources to perform them. But at the same time, alternative assessment needs to take many important aspects into account.

Inadequate data challenges textile chemical management and LCA (Roos, 2016). While chemicals related to energy production are quite comprehensively compiled in LCI databases, chemicals related to textile products are commonly just assessed qualitatively. For example, Roos (2016) mentions LCA studies for textile products where the toxicity impacts are not included in the reports due to the fact that the inventory data for textile chemicals were not fully complete. Another challenge is that even if all chemicals used in the processes were to be known, the characterisation factors needed to calculate the impact are still unknown for many substances.

2.5.3 Combining Life Cycle Assessment and Risk Assessment

There are several ways to combine RA and LCA. Each option of combination has different strengths and uncertainties. This section will go through examples of some different views on combination encountered in the literature.

Generally, one of the differences between LCA and RA is that while LCA mainly calculates relative impact values, RA mostly focuses on calculation of absolute values of exposure (Tsang et al., 2017). Tsang et al. (2017) recommends that LCA and RA are combined at the methodological level, and present three different levels of integration: site-generic, site-dependent and site-specific. They also include the option of performing the two assessment tools separately and instead combining the results. These ways of combining the methods relate to the geographical boundaries and modelling in the study. Site-generic combination uses steady-state assumptions for generic environments and settings, site-dependent combination instead uses dynamic fate and exposure models, and site-specific combination is done with a specific emission setting. Site-generic combination can be an LCA that compares potential impacts, whereas site-specific combination can be used to yield absolute impacts for human health. For the combination of results from LCA and RA as separate tools, Tsang et al. (2017) and Linkov et al. (2017) suggest using for example, multi-criteria decision analysis (MCDA) as a weighting method. Linkov et al. (2017) argues that integrating LCA and RA on a methodological level could result in the strengths of the two assessment tools being undermined. Instead their suggestion is to use LCA and RA as two separate tools and that the result of these studies then can be integrated. For comparison of LCA and RA, a difficulty is the different scopes of the two tools, since LCA relates the impacts to a functional unit while RA are based on exposure scenarios. A type of site-specific integration can be to do the RA in such a way that it matches the LCA scope (Tsang et al., 2017).

Another way of combining these two methods is through the use of CFs for the specific chemicals studied in the system (Lin et al., 2017). According to Breedveld (2013), utilising information and toxicological data from RA in the LCIA is the most common combination of LCA and RA. RA usually only focuses on one chemical, but by calculating CFs through the RA, and then using these in the LCIA, a better view of toxicological impacts from different pollutants can be achieved (Lin et al., 2017). Fantke et al. (2017) explains that CFs can be determined with information regarding the exposures and the effects to humans and the environment using the USEtox model, which is one of several models available to calculate toxicity in LCIA. The USEtox model calculation is based on integrating chemical exposure routes to the receptor. The calculation of the characterisation factor consists of three main factors: fate, exposure and effect. The results for human toxicity impact are given in CTUh (comparative toxic units) while for the environment, the result is represented as ecotoxicity and expressed in CTUe. CTU is used to express number of cases per kg mass of chemical. Uncertainties factor of the USEtox model in calculating CFs for human toxicity is in the range 100 - 1000, while for ecotoxicity, the factor is between 10 - 100 (Rosenbaum et al., 2008)

When RA is done for a specific exposure scenario, several RAs would need to be added up to get the full view of potential risks in a chemical's or product's life cycle. Kuczenski et al. (2011) propose that RAs should be made more "life cycle aware" by adapting the concept of process flow models used in LCA. Kuczenski et al. (2011) further argues for a more precautionary approach in RA, with more focus on inherent characteristics of chemicals. It is also suggested that LCA can be made more "toxics aware" by also tracking and characterising the intermediate flows of chemicals within manufacturing processes, not just the emissions that currently is the main focus. By including more information on toxicity (of intermediate flows) in LCA, it could

put focus on processes and product systems that are or could be problematic, instead of only certain problematic emissions.

Breedveld (2013) and Walser et al. (2017) also recommends a combined method which focuses on integrating a life cycle perspective in RA, called Life Cycle Based Risk Assessment (LCBRA). LCBRA can be used to assess risks throughout the different stages of a chemical's whole life cycle (Breedveld, 2013). However, as LCBRA can lack information on the exposure on a population level, Walser et al. (2017) recommends to also conduct an LCA to complement the results for decision making process (Walser et al., 2017).

A method to compare LCA and RA results is by comparing results expressed with the same unit. Human health effects can be expressed as Disability-Adjusted Life Years (DALYs) (Kobayashi et al., 2015a). There are different methods to calculate DALYs in LCA, which uses different characterisation factors. The ReCiPe method also uses three different cultural perspectives: egalitarian, hierarchist and individualist (Kobayashi et al., 2015b). Kobayashi et al. (2015b) strongly recommends that DALYs from LCA and RA should not be directly compared if the derivations are not consistent between the two assessment tools. It is also important to consider for which population the DALYs are meant to represent. For example, global average DALYs could be an overestimation of human health impact in developed countries since they might have better healthcare system compared to developing countries. Environmental effects could, in a similar fashion, be expressed with the unit potentially disappeared fraction of species (PDF) (European Commission, 2012).

A combined use of both LCA and RA is often recommended to get a holistic view of the system (Kobayashi et al., 2015a). A reason for deriving DALYs from both LCA and RA is that the derivation of DALYs from LCIA midpoint results does not always take all types of environmental impact into account. By performing an RA, some of the impacts missed by the LCA might be possible to take into account. DALYs can be used as a way to directly compare results from LCA and RA, but for this to be possible, the assumptions used to calculate the DALYs must be consistent for the two assessment methods.

2.6 AkzoNobel's Current Sustainability Work

AkzoNobel is currently conducting work as part of their commitment towards sustainability. Eco Premium Solutions (EPS) is a method used to develop products to be more sustainable by comparing products by AkzoNobel with other products in the market, based on criterion for health, safety and environment (AkzoNobel, 2017a). This method considers the life cycle of the products. AkzoNobel has also applied "priority substance management" which focus on managing hazardous chemicals. Through this approach, they reviewed their products and prepared for changing of regulation in the future (AkzoNobel, 2017d). Regarding the carbon footprint along the value chains of their products, based on the Resources Efficiency Index data in 2017, there were a slight decrease from previous year (AkzoNobel, 2017b). There was also reduction of emission per thousand kg of product. During last year, AkzoNobel also showed their commitment in reducing carbon footprint by winning the Cefic award which is a recognition for best Europe chemical company in term of health, safety and environment standards (AkzoNobel, 2017c).

2.6.1 Information About the Case Study

As mentioned in the introduction, chemical A and B are two chemicals produced by AkzoNobel and are for example used in softener manufacture. Both chemical A and B can be found on bluesign's restriction list (bluesign® technologies ag, 2017). bluesign have put chemical A under a usage ban. Chemical B is not under usage ban, but has limit values for the different usage ranges (the specific values cannot be included here due to the confidentiality surrounding chemical A and B). However, these usage bans refers to direct use of the chemicals on textiles articles, and AkzoNobel is not aware of anyone using chemical A and B as such directly on textile, and has not REACH-registered such use in EU (AkzoNobel, 2018, personal communication). For example, chemical A is only allowed to be used as intermediate raw material to produce other chemicals in the EU.

Chemical safety assessments have already been made on chemical A and B on behalf of AkzoNobel (AkzoNobel, 2013; AkzoNobel, 2017). These previous assessments looked at several different applications that chemical A and B are used for. The RA on chemical A included the application in textile softener and safe use for workers (with adequate safety measures), for the consumer and the environment was demonstrated. The chemical safety report (CSR) for chemical B did not include application in textile softener. These previous assessments have mainly been communicated internally within AkzoNobel, but now the idea is to (eventually) communicate the result to the downstream stakeholders, such as the softener producer – to show them how assessments like these work, what protection equipment etc. that they need to use in order to continuing ensuring safe use, and identifying hot spots where action can be taken to reduce the exposures.

3. Method

3.1 Technical System

Figure 3.1 presents the involved actors for the studied value chain in this case study. The whole value chain was assumed to take place in China.

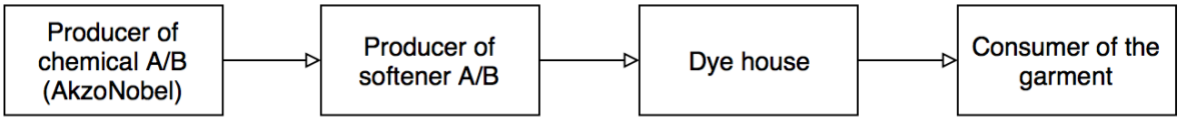

Figure 3.1: Involved actors in the softener value chain.

The focus of the study was on the use of softener in textile wet treatment (taking place at the dye house). Softeners can be used on both yarn, fabric and garment. There are different types of machines and methods used, in the case study the focus was on two methods called padding and dipping, based on the information from the softener producer.

For information about the involved processes, personal communications have been made with the softener producer throughout the duration of the thesis. An LCI questionnaire which was already designed by AkzoNobel was used to collect data and information from the producer of the softener. Still, the information received about the downstream processes did not cover all data information requirements, and therefore assumptions had to be made.

3.1.1 Chemical Properties

Table 3.1 below shows a general description of chemical A and B. As can be seen, both chemicals are volatile, completely miscible and readily biodegradable. The physical state of both chemical A and B at 20˚C and 1013 hPa is liquid (ECHA n.d.-b). They are very similar when looking at this general description, but there are some differences. For example, the vapor pressure of chemical B is significantly higher than the vapor pressure of chemical A.

Table 3.1 General properties of chemical A and B.

Property	**Chemical A**	**Chemical B**
Molecular weight	90-120 g/mol	
Vapor pressure	0-10 Pa	20-30 Pa
Boiling point	220-250°C	200-230°C
Water solubility	Completely miscible	
Partition coefficient octanol-water (logKow)	-1.5 - (-1.0)	
Biodegradation	Readily biodegradable (OECD 301)	

Chemical A and B are reacted with other chemicals to form a new substance that makes up the softener; softener A and softener B, respectively. The amount of chemical A and B in the softener production differs between the two softeners. As the amount of chemical A and B residues in the softener was not known, it was assumed to be 10 ppm. While this is a simplification, preliminary results from a confidential analysis done by AkzoNobel on yarn samples validate this assumed average level of residues. There is a concern that softener A and B might cleave back into chemical A and B, but if this occurs, and if so to what extent, is currently not known.

The softener product is in the form of flakes (Softener producer, 2018, personal communication). These softener flakes are put into bags and sold to the customers. Softener is typically industrially used in what is called the dye house, which is the wet treatment part of textile production. Yarn, fabric and garment are treated with softener, to give the fabric a pleasant feel for the wearer.

3.1.2 Process Descriptions

When the softener is used, the softener flakes are first diluted in water, usually to around 10% solution (Softener producer 2018, personal communication). How much softener that is then used to treat the fabric can differ, for example depending on the type of softener, type of fabric and type of process that is used. To use the softener, there are two types of processes that are used in our case study: padding and dipping. The softener producer recommends the following: padding uses 2-3 g softener/L water and dipping 3-8 g softener/kg fabric. In the RA exposure assessment 3 g softener/L was used for padding, and 8 g softener/kg fabric for dipping. The LCA was based on softener use of 5 g softener/kg fabric (dipping method). According to the softener producer, the dye house often uses less softener than their recommended dose, meaning that the calculated exposure might be higher than the actual exposure. The amount of water used also differs between padding and dipping. Based on the information received from the softener producer, it is assumed that padding uses 0.8 L/kg fabric and dipping 8 L/kg fabric. For treatment of yarn and garment, dipping is used. For treatment of fabric, either padding or dipping could be used.

The water and softener in this water will then be absorbed by the fabric (Softener producer 2018, personal communication). According to the softener producer, during padding all the water and softener is absorbed, whereas using dipping process about 50% of the water and softener will be absorbed. The remaining water and softener will be sent to wastewater treatment. The wet fabric will then be dried (during which the water is removed from the fabric, but all the softener is assumed to stay in the fabric), and then sent to the next step of textile production.

For the RA, the following assumptions have also been made regarding these processes (unless stated otherwise, these are based on information from the softener producer (2018, personal communication)):

- The softener that is already absorbed by the fabric in one step will not dissolve again into the water in the next step. For example, the softener that is absorbed onto the yarn will not dissolve into the water again when the fabric is treated with softener. This means that the calculated amount of chemical A and B in the final garment might be higher than in

the real scenario, as chemical A and B are soluble in water and therefore it could be expected that some of the residues would dissolve during the treatment process.

- The water use of 0.8 L/kg fabric in the padding process is based on an 80% weight increase of the fabric during this process and that this process has no output of water (i.e. all water is absorbed by the fabric). This would mean that the recommended dose for padding is 1.6-2.4 g/kg fabric (2-3 g/L multiplied by 0.8 L/fabric). The water use in dipping process is based on a liquid ratio of 1:8 that is usually used (which would correspond to 0.4-1 g/L) .
- As mentioned, padding or dipping could both be used to treat fabric. In the RA (for the exposure to the consumer), it was assumed that dipping is used, as that would result in a higher concentration of residues in the final garment. (In padding, 2.4 g/kg of softener is used, and all of this is assumed to be absorbed by the fabric. In dipping, 8 g/kg is used, and if 50% of this is absorbed the fabric will have absorbed 4 g/kg. With these assumptions, dipping will hence give a higher exposure both for the consumer as well as the environment.)

3.2 Risk Assessment

3.2.1 Goal and Scope

The aim of this RA was to assess the risk to human health throughout the life cycle of chemical A and B when used in textile softener. Risks to the environment were also assessed, though not in focus. The focus was the consumer, to see if there is an expected risk from clothes containing residues of chemical A. Workers were also considered. The main safeguard subject was the consumer wearing the garment; in this case the most sensitive being pregnant women, due to the reproductive toxicity classification. Small children were accounted for as well. Since the reprotoxic effects were the main concern, the focus was on these systemic effects, whereas local effects were not considered as important for this particular case. The exposure of consumers to the same chemicals via other products was also considered with the intention to more accurately determine if the consumer is at risk. This RA was done with guidance from the ECHA guidelines on CSA (ECHA, n.d.-d).

The risks along the corresponding life cycles of chemical A and B was assessed. Possible exposure to these two chemicals to workers, consumers or the environment might occur in the manufacturing of these substances, in the production and use of the softeners, as well as the consumer use of the garment and disposal of the garment. Exposure to consumers when the consumer is using fabric softener when washing their clothes at home was not included in this RA, as softener A and B are industrial textile softeners and are therefore not sold to households. As neither of these chemicals are persistent or bioaccumulative (ECHA, n.d.-c), uptake through food and plants was not assessed. Based on that the main focus of this RA were the systemic effects to the consumer, this was prioritised and the exposure to retailers was excluded due to time constraints.

3.2.2 Conceptual Model

Based on the chemical properties of chemical A and B and the process information, figure 3.2 and 3.3 below shows a simplified conceptual model for chemical A and B when used in textile softeners. It demonstrates where the residues is expected to end up and who might be exposed throughout the different life cycle processes.

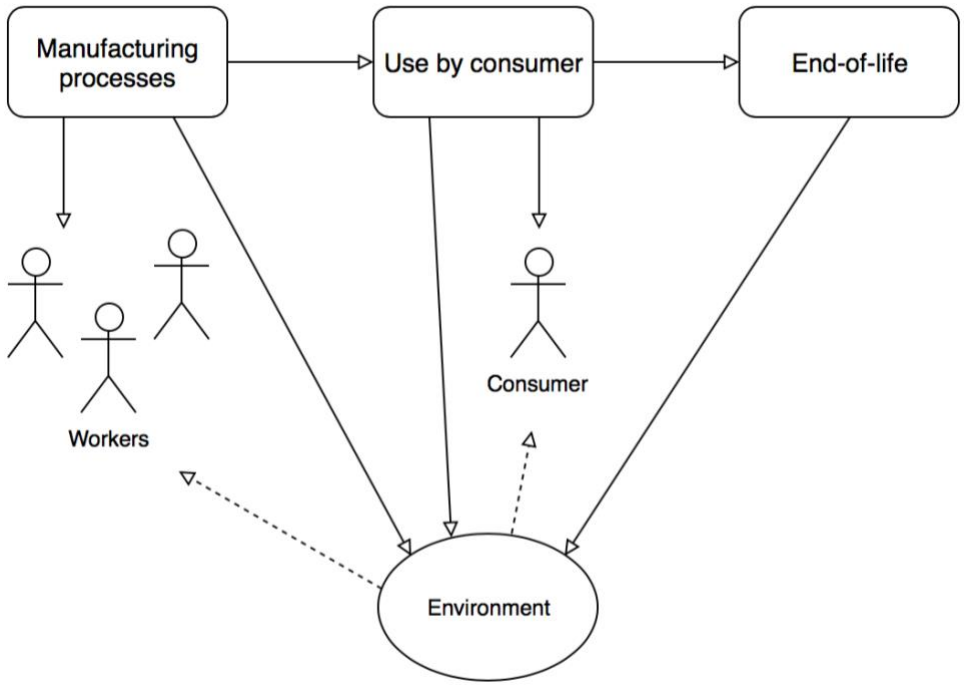

Figure 3.2. Conceptual model of the life cycle of the studied chemicals in textile softener application. Arrows depict exposures.

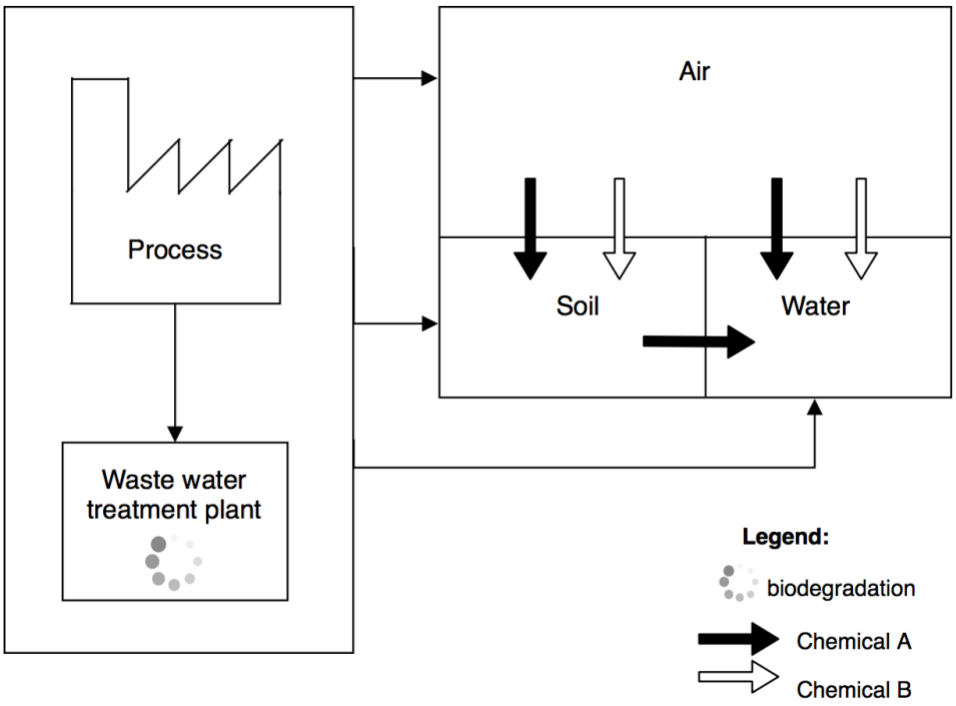

Figure 3.3 Conceptual model of the environmental fate of the studied chemicals.

The environmental box in figure 3.3 demonstrates how chemical A and B are expected to move between the environmental compartments after emission to these. With chemical A, all emissions are assumed to eventually end up in water. This is also expected for chemical B, except for the emissions to the terrestrial compartment. Because chemical B binds strongly to soil, limited exchange from soil to water compartment is expected (AkzoNobel, 2017). Emissions of chemical B to soil are hence expected to remain in the soil.

Figure 3.2 indicates who is expected to be exposed to the chemicals. Based on this conceptual model and the scope of the thesis, the safeguard subjects of interest in this case study are mainly the consumer of the garment, but also the workers involved in the production of the chemicals, production of the softener and use of the softener. In these industrial processes, the workers can be exposed through inhalation, dermal contact or eye exposure. The exposure levels will of course depend on, for example, the process equipment and on the personal protection equipment used. The consumer can mainly be exposed to the chemical residues through dermal contact, although inhalation might be possible, as well as oral intake for small children. Another exposure pathway can be drinking water. Due to the biodegradation of chemical A and B, the risks through some exposure pathways might not be as relevant, since the substances is likely to degrade to lower exposure levels in wastewater treatment plant.

3.2.3 Hazard Assessment

The Predicted No Effect Concentrations (PNECs) are the derived “safe-level” for the environment (for example aquatic toxicity) and Derived No Effect Levels (DNELs) are for humans. These threshold values are derived from different points of departure, usually No Observed Adverse Effect Level (NOAEL), Lowest Observed Adverse Effect Level (LOAEL) or

a benchmark dose (BMD). These values can be obtained from animal studies, where the NOAEL represents the dosage that did not result in a harmful effect in the studied animal and the LOAEL is the lowest dosage that resulted in a statistically significant harmful effect. Using assessment factors, the NOAEL or LOAEL is extrapolated down to a DNEL, a level that represents the dose a human can be exposed to that will not cause any adverse effects. In other words, if a person would be exposed to higher concentrations than the DNEL, there is a risk of adverse effects to occur. One can also use a BMD to derive the DNEL. Dose-response modelling can be used to find dose levels that corresponds to certain effect levels (EPA, 2012). The BMD lower confidence limit (BMDL) represents the lower limit of a one-sided 95% confidence interval on the BMD.

DNELs and PNECs were not calculated as part of this study. Instead, DNELs and PNECs used in the previous studies done by AkzoNobel (2013; 2017) were used, with updated values from the ECHA REACH registration dossiers where available (ECHA, n.d.-c).

3.2.4 Exposure Assessment

3.2.4.1 Workers

To calculate the exposure to workers, the European Centre for Ecotoxicology and Toxicology of Chemicals Targeted Risk Assessment (ECETOC TRA) model version 3.1 was used (ECETOC, 2017). For this, Process Categories (PROCs) were used based on a previous RA done on chemical A (AkzoNobel, 2013). PROCs describes the activities done by workers, which will have different exposure potential for the workers, with the intention to "*support harmonised and consistent exposure assessment across sectors and supply chains*" (ECHA, 2015).

To calculate the exposure of chemical A and B to workers, the following properties needed to be added into ECETOC TRA:

- Molecular weight
- Vapour pressure
- Water solubility
- Partition coefficient octanol-water (Kow)
- Biodegradability test result

Seen in the table below are the ranges ECETOC TRA uses for substance vapour pressure. Both chemical A and chemical B are assigned low fugacity by ECETOC TRA despite a quite big difference in vapour pressure. Thus, the results of the ECETOC TRA exposure assessment will not reflect this difference in vapour pressure.

Table 3.2 Intervals used by ECETOC for vapour pressures (ECETOC, 2017).

Vapour pressure (kPa)	**Fugacity**
< 0.00001	Negligible
≥ 0.00001 - < 0.5	Low
≥ 0.5 - ≤ 10	Medium
>10	High

See table in section 8.2 (Appendix) for a short explanation about the PROCs used in this RA. These are the same for chemical A and B, as the processes involved were assumed to be the same. The Local Exhaust Ventilation (LEV), personal safety equipment, duration of activity, concentration of substance in preparation and state (solid or liquid) of substance were also chosen as the ones previously used in the RA on chemical A by AkzoNobel (2013). In ECETOC TRA, different settings can be used for the PROCs. For example, ECETOC takes into consideration the type of setting (industrial/professional), dustiness, duration of activity and level of personal protection equipment. The settings that were used for each PROC is available in the confidential appendix.

In the previous RA on chemical A, two different (non-consumer) uses of softener were assessed: use at industrial site and use by professional workers. ECHA (n.d.-e) define the latter as activities taking place at construction sites, workshops, or other places that is not an industrial site. In this RA, only use at industrial sites was assessed as that was considered most relevant, based on that textile wet treatment is regarded as "use at industrial site" by ECHA (2015).

3.2.4.2 Consumers

Based on the highest recommended dosage of softener, it was first calculated how much softener that is used and absorbed on the yarn, fabric and eventually final garment. Then based on how much of chemical A and B residues that are assumed to be in the softener, it was derived how much chemical A and B that can be expected to be on the garment once it reaches the consumer.

The following assumptions were based on Meesters et al. (2018), and used to calculate the exposure to the consumer when wearing the clothes:

- Default product amount is 1 kg for adults. This default value is based on the weight of summer clothes and winter clothes (not including thick sweaters on top of the other clothes).
- Default skin-contact factor is 0.8. This is the fraction of the clothes that will be in direct contact with the skin (80%).
- Meesters et al. (2018) also uses something called leachable fraction, which is the *"fraction of a substance in a laundry product that is able to leach from clothes to the skin of the person wearing them"* - (Meesters et al., 2018, pp 80). Previously, they had 50% of the residual product amount assumed to migrate from the clothes to the skin, but a new default is set to 10%. Hence, in this RA it was assumed that 10% of chemical A and B in the clothes can migrate from the clothes to the skin.
- The body weights used in this RA for consumer exposure are based on Biesebeek et al. (2014). Their default values for body weights are 64.1 kg for women and 4.5 kg for children (assuming that the child is between 1-3 months old). One should keep in mind that the consumer of concern is pregnant women, due to the risk of developmental toxicity, and so the weight could perhaps be higher. However, the lower the body weight used, the lower the DNEL will be (since the unit is mg/kg bw/day) – and so, using this default weight helped form a worst-case scenario.
- To calculate the risk quotient for local dermal exposure, the amount of chemical A and B in mg/kg fabric was converted into mg/cm^2 fabric. This was done using the specific

surface area of cotton fabric given in Meesters et al. (2018) of 20 cm^2/g. Hence, it was also assumed here that the assessed 1 kg fabric is made of cotton.

- 5.4 kg of laundry is the average weight of clothes washed per full load (in washing machine by consumer), with a water use of 6.2 kg water per kg fabric (Roos et al., 2015b). This was used to estimate possible emissions of chemical A and B to water from the use phase.

Equation 1 below shows how dermal exposure was calculated:

*Dermal exposure to chemical A or B (mg/day) = softener added (mg/kg fabric) * absorption rate * level of chemical residues in softener * weight of clothes (kg fabric/day) * skin factor * leachable fraction (1)*

Initially, oral exposure might not seem relevant when thinking of clothes, but it becomes a possible exposure pathway when considering exposure to children, as they tend to put things in their mouth. Since chemical A and B are water soluble, the child might be exposed to these residues through the saliva when chewing on the fabric, and it was hence assumed that all chemical A/B residues in the clothes can migrate from the fabric (instead of the 10% used for dermal exposure). If the exposure is calculated on the basis of 1 kg of textile, which of course is a worst-case assumption when it comes to a small child, especially since they will not stuff the whole sweater in their mouth, the daily exposure would hence be the amount of residues of chemical A/B in 1 kg of clothes.

The inhalation exposure was calculated based on volumes of air of 2 m^3 and 20 m^3, which represents the air in close proximity to a person ("breathing zone") and the default room volume, respectively (ECHA, 2016b). It should be noted that using the air volume of 2 m^3 is an overestimation of the exposure, so this was chosen to get a maximum exposure. To further make a worst-case scenario, it was assumed that all chemical A and B residues in the fabric would evaporate (and expose the consumer). The exposure through inhalation is calculated in the following manner:

Exposure (air concentration) = chemical A/B residues in fabric / air volume (2)

In reality, the consumer can also be exposed to other textiles that have also been treated with softener A or B. Chemical A is also used in the manufacturing of body lotions and similar products, which is also a potential exposure route. To take this additional exposure into account, the scale of these exposures in order for the risk quotient to be equal to 1 were calculated (this was done on textile products, assuming that these other textiles contains the same amount of chemical A/B residues as our case). For inhalation and exposure through drinking water, this was also done by calculating backwards. For the exposure to chemical A and B by drinking water, a worst-case was used by taking the concentration of the water after using the softener in textile wet treatment, without any wastewater treatment or dilution. This was done using the equation below:

*Concentration of chemical A/B in water = added softener to water / water use * level of chemical A/B residues in softener (3)*

3.2.4.3 Environment

As mentioned, the emissions to the environment were not the focus of this RA and were only included in regard to emissions to water, from using the softener and from washing the garments. Possible exposure to air and soil were assumed negligible compared to these water emissions. For the emissions to water (from the use of softener and use of garment phases), standard dilution factors from ECHA guidance document R16 (ECHA, 2016a) were used: 10 and 100 for release to freshwater and marine environment, respectively. These were used instead of site-specific data, since that was not available. Regarding emissions to water, the concentration without wastewater treatment plant (WWTP) was first considered, to see if there was reason to expect aquatic or human toxicity. In case the risk was shown to be uncontrolled, whether wastewater treatment would efficiently reduce the risk was assessed. For a worst-case scenario, it was assumed that the water not absorbed in textile wet treatment was not re-used (in a continuous process) and was instead discharged, with no wastewater treatment.

To make a worst-case scenario for environmental exposure from the consumer washing the clothes, it was assumed that new clothes are washed before being worn, hence containing maximum amount of chemical A/B residues. Furthermore, it was assumed that all of these residues were washed out from the fabric. As mentioned, the average full load of clothes in washing machine is 5.4 kg (Roos, et al., 2015b). The water used, based on 6.2 kg water/kg fabric, would hence be 33.5 kg of water. The concentration in the water out from the washing machine would then be calculated using equation 4. This concentration was then adjusted with dilution factors of 10 and 100, for freshwater and marine water, respectively.

Chemical A/B in washing water = Chemical A/B in fabric / water use *(4)*

By the time the clothes are disposed of, it was (in this RA) assumed that the chemical A/B residues in the fabric either has been absorbed by the consumer and/or washed out during the significant number of washes during the lifetime of the garment.

3.2.5 Risk Characterisation

The risk characterisation ratios (RCRs) were calculated based on the following relation:

RCR = Exposure / DNEL *(5)*

They were calculated for workers (for the different PROCs separately) and for different exposure routes for consumers.

For the environment, the RCRs were calculated using equation 6.

RCR = Exposure / PNEC *(6)*

This was done for aquatic organisms, from diluted wastewater from textile wet treatment and from the consumer washing (new) clothes.

3.2.5.1 Robustness Assessment

To assess how robust the results are, some backward calculations were made. This departed from the systemic long-term exposure to chemical A for women, since this was the main focus of this case study and the DNELs for chemical A were lower than for chemical B. Equations 7-9 below describes how the required amount (which would give RCR=1) residues of chemical A in softener and the required amount of softener content in the fabric were calculated, if the residue level would remain the same.

Chemical A residues required in fabric = exposure of chemical A required / leachable fraction *(7)*

Chemical A residues required in softener = chemical A residues required in fabric / softener in fabric *(8)*

Softener required in fabric = chemical A residues required in fabric / level of chemical A residues in softener *(9)*

The previous exposures were based on the assumption that the woman is wearing 1 kg of (new) clothes per day. Of course, she is also exposed to other textile products, like bed linen, towels, furniture, etc. Assuming that these textiles contain the same amount of chemical A residues as the clothes, i.e. 10 ppm, this would be the required exposure:

Other textile products = exposure required / chemical A residues in textiles *(10)*

As mentioned in the background, there is a concern that softener A and B might cleave back into chemical A and B. At the moment, there is limited knowledge about the softener and its molecular structure. Therefore, it was accounted for using the assumption that maximum cleavage occurs, to assess what the resulting RCRs would be.

For inhalation the required amount of fabric needed to get RCR of 1 (long term, systemic, inhalative DNEL for chemical A) was calculated, for an air volume of 2 m^3 ("breathing zone") and 20 m^3 (default room volume), respectively. Keep in mind that this was based on the assumption that all chemical A residues would evaporate, and that this would be completely new fabric (hence containing maximum amount of free chemical A).

How much water a person would need to drink (directly from the textile wet treatment outlet) in order for the RCR to be equal to 1 was calculated using equation 11.

*Required amount of water = required exposure / chemical A concentration in water = Oral DNEL * body weight / chemical A concentration in water* *(11)*

If calculating backwards to how much fabric the child would need to put in its mouth during one day in order for the risk to be uncontrolled, this amount would be:

Fabric required = required exposure / chemical A residues in fabric *(12)*

3.3 Life Cycle Assessment

3.3.1 Goal and Scope

The purpose of this LCA was to identify which option that is preferable from environmental point of view for the future use of chemical A and B in softener production; comparing the current use scenario where both chemical A and chemical B are used, with an alternative scenario where only chemical B is used. In this second scenario, chemical A is not used and is instead incinerated. The specific goals were:

- Identify the preferred option, continued or discontinued use of chemical A
- Identify the uncertainties and methodological choices that may affect the comparison between two chemical substances.

The focus of the case study was the use of chemical A and B for fabric softener production. The LCA comparing chemical A and B was of cradle-to-grave type and was done with guidance from the ISO standards. Social and economic impacts was excluded from the LCA, as focus was on environmental aspects.

GaBi Professional software (version 8.1) was used for computing LCA results in this case study. The input data and information used in this study was collected from AkzoNobel database, Ecoinvent version 3.4 and information from the softener producer.

3.3.1.1 Functional Unit

The functional unit (FU) used in this study was 2 kg of softener, which corresponds to treatment of 42-131 kg of fabric (67 kg of fabric if using a softener dose of 0.5% in dipping on yarn, fabric and garment). The FU was chosen due to the fact that while different softeners usually have different properties and hence do not give the exact same result in the textile product, the information on softener dosage recommendations received from the softener producer in this case does not indicate a difference in performance between softener A and B. Thus, the same amount of produced/used softener will in this case result in the same amount of treated textile.

3.3.2 System Boundaries

This study was conducted as an A-LCA, cradle-to-grave. The main life cycle of chemical A and B is illustrated in figure 3.4. Scenario 1 to the left represents the involved processes for using chemical A and B to produce softener A and B, respectively. Scenario 2, to the right, represents the processes for when only softener B is produced, and chemical A is incinerated. There are then additional options for this second scenario, where the heat generated from incinerating chemical A can be used to replace an alternative fuel or energy source. LCA of chemical A and chemical B in softener includes all phases in the life cycle (limited to the impacts allocated to the softener, as mentioned further below): raw material production, softener A and softener B production, use of softener in textile wet treatment, use of garment and incineration of garment. For electricity production, the data were based on the energy production of the countries where the plant and factory are located, which are presented in more detail in the geographical boundaries section.

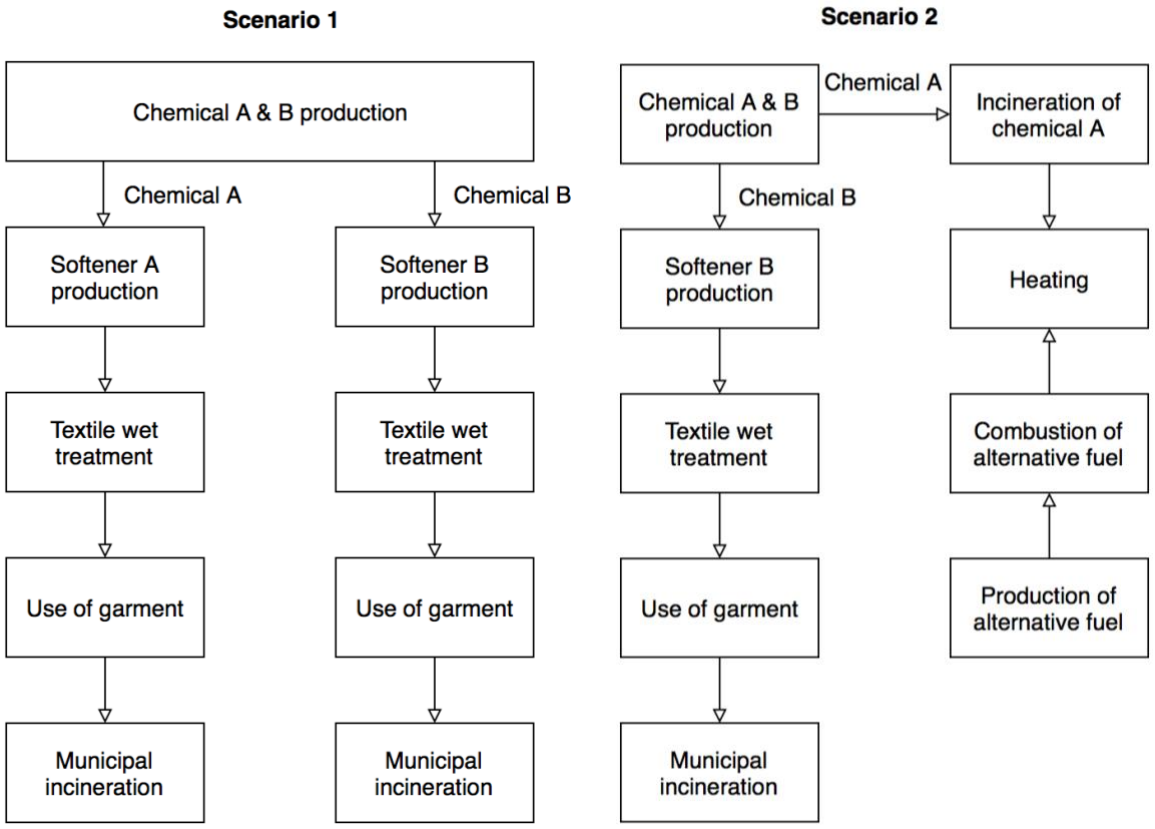

Figure 3.4 Flowchart of the analysed systems in the case study.

To analyse the other options for the second scenario, system expansion was used for energy recovery. The generated heat from incineration of chemical A were in these scenario options used to replace the same amount of energy as produced from coal or wind power. It is important to note that in this study only the softener life cycle was included for the whole life cycle without considering the additional impact from the textile. The inputs and outputs of the system were allocated to the amount of softener and not to the corresponded amount of treated textile. For the chemical manufacturing, all inflows and outflows were included in the LCI, except possible emissions of chemical A and B. In softener production and textile wet treatment, water use and wastewater was excluded from the system. For the residential washing no water use or energy requirements was included as that was allocated to the textile. For the end-of-life, incineration of the softener, and not the textile, was considered.

3.3.3 Technical Boundaries

Chemical A and B production (see process “chemical A & B production” in figure 3.4) is a multi-output process with several other chemicals produced. They are produced at a fixed ratio, so it is not possible to increase production of one of the chemicals without increasing the production of the other chemicals. In the same way, to stop the production of chemical A, production of all these chemicals would need to cease. This is why chemical A is still produced in scenario 2. However, all other outputs have been omitted from this LCA, since it focused on chemical A and chemical B.

Scenario 1 includes parallel use of chemical A and B, contributing to the FU with 1 kg of softener A and 1 kg of softener B. Within this system, the impact of softener A can also be compared to softener B (on the basis of 1 kg of softener). Scenario 2 include the continued use of chemical B to fulfil the FU (i.e. 2 kg of softener B), while the use of chemical A is discontinued and the chemical is instead incinerated. The amount of chemical A that goes to incineration corresponds to the amount of chemical A produced (in process "chemical A & B production") to generate the amount of chemical B needed for 2 kg of softener. In scenario 2 three options were assessed: i) without energy recovery, ii) with energy recovery to replace coal, and iii) energy recovery to replace wind energy. Options ii and iii covers the two extremes and as such the full range of possible impacts from this system expansion was captured.

3.3.4 Time Boundaries

Most of the data for chemicals production process were collected from AkzoNobel's 2016 database. The inventory data from the Ecoinvent database were mainly data from 2014. Data from the softener producer were collected through personal communication in 2018 and represent the current situation.

3.3.5 Geographical Boundaries

The data for production process of the chemicals is based on database from AkzoNobel's plant in China. The softener manufacturing process that was analysed in this study is also located in China. Based on information from the softener producer, the other chemicals are produced in different locations with estimated distances around 50-100 km from the softener production plant. For the use phase of the garment, it was assumed that the garment will also be used by consumers in China as well as waste management of the garment.

3.3.6 Life Cycle Inventory

Data for the background processes were taken from the Ecoinvent database, while the foreground was inventoried with a questionnaire that was filled out by the softener producer. A report by Roos et al. (2015b) was also used to fill the information gap related to energy requirements in textile wet treatment process. For direct chemical emissions, it was focused on chemical A and B. However, emissions from the production process of chemical A/B were excluded in the model.

In order to calculate the direct emissions of the chemical A/B, emission factors (EF) were applied, based on the environmental release categories (ERC) in the previous RA report from AkzoNobel as presented in table 3.3 below (AkzoNobel, 2013; ECETOC, 2017). The EFs that were used in this report are based on realistic worst-case scenarios. The EFs are applied on the input. For example, 2% of input of chemical A used to produce softener A is assumed to be emitted to water. For the textile wet treatment, 50% of the input was assumed to be emitted, and then 50% of this to be released to air and the other 50% to water. This was an adjustment of the release factors, based on the calculation in RA exposure assessment (50% of softener applied sticks to the fabric), as otherwise using these factors as they are means nothing is left on the product.

Table 3.3 ERC emission factors to air and water.

Stage	ERC	Default release to air from process	Default release to water from process
Manufacturing of chemical	1	5%	6%
Production of Softener	6a	5%	2%
Textile Wet Treatment	5	50%	50%

The EFs do not include emission abatement. For emissions to water, biodegradation of chemical A and B were however accounted for in the model, more about this in the next paragraph and in section 4.2. Calculation of emission to soil was excluded in this LCA.

While a WWTP process was not included (in the model) after production of softener, textile wet treatment and residential washing, in terms of energy requirement or general output, it was accounted for by adjusting the emissions of chemical A and B (to water) according to the biodegradation rates. For the softener it was assumed that 20% would wash out from the garment during each wash (by the consumer). Water use in textile wet treatment was not included, but it could be so in a further developed model. In residential washing, water use was not included since it was allocated to the textile not to the softener.

3.3.7 Life Cycle Impact Assessment

The impact categories included were: climate change, acidification, eutrophication, ecotoxicity, human toxicity and ozone layer depletion. For climate change, acidification, eutrophication, and ozone layer depletion ReCiPe midpoint (v 1.08) were the characterisation method used. Ecotoxicity and human toxicity impacts were calculated with USEtox (v 2.01).

New characterisation factors were calculated for chemical A and B with the USEtox 2.01 model. In current USEtox database, the characterisation factor for ecotoxicity for chemical A and chemical B were already available. The characterisation factors for human toxicity were calculated with the USEtox ecotoxicity characterisation factors substance data for fate and exposure parameter and effect data from the RA. The toxicity data inventoried in the RA was used to obtain the effective dose where 50% of the population show the effect (ED50), according to the USEtox manual (Huijbregts et al., 2010). The NOAEL data chosen to calculate ED50 for chemical A and chemical B in this case study were done using the lowest numbers found in several previous studies. ED50 was directly calculated by multiplying the NOAEL with factor of 9.

For the DALY calculation, the ReCiPe characterisation factor was used for conversion from climate change and ozone layer depletion impact to human health impact. Human toxicity with cancer and non-cancer were also converted to DALY with conversion factor 2.7 DALY and 11.5 DALY, respectively, as described in the USEtox Documentation (Huijbregts et al., 2010)

3.3.8 Assumptions and Limitations

During the collection process of data, it became clear that information for some processes were hard to obtain. Due to the availability of information and time limitation, there are some assumptions and exclusions in this study which are listed below:

- Due to limitation of the information, only transportation of the raw materials used in the softener production was included and other transportations were excluded (assumed negligible).
- Related to steam/heat production using straw boiler in the softener manufacturing, the available data was collected from Denmark Boiler Heat from Ecoinvent data. All the electricity for the processes was modelled as supplied by general electricity grid in China.
- Based on information from the softener producer, softener A can be diluted with cold water while for softener B, hot water is needed for the dilution process. Since there was no further information related to the hot water needed for softener B, it was assumed that the heating needed is similar with the heating needed for dyeing weave orange in jet dyeing machine based on general data (Roos et al., 2015b). The dyeing machine was heated with the boiler at the softener manufacturing plant.
- Due to data limitation in textile wet treatment process, the energy needed in this step was based on a report by Roos et al. (2015b). Amount of electricity used in the model was assumed to be similar with data for dyeing weave orange process in jet dyeing machine. This process was chosen out of several dyeing processes available in the report since it included softener in its inventory data. The number was scaled up based on the amount of softener used in that process and compared to amount of softener A/B in this case study.
- In scenario 2 the LCA assesses the substitution of softener A with softener B, with several options: without energy recovery and with energy recovery to replace energy from coal and wind.
- In the textile wet treatment, the use of softener on yarn, fabric and garment was not modelled as three separate processes, instead these processes are modelled as one process.
- The emissions of chemical A and B from different stages in the softener life cycle were based on realistic worst-case scenarios, using ERCs factors. For manufacturing of chemical A/B, the emissions were excluded.

4. Result

In the following sections, the result from the case study will be presented, divided into the two assessments, RA and LCA. Thereafter a recommendation for combined framework of LCA and RA, based on the scope and result of this case study, is presented.

4.1 Risk Assessment

4.1.1 Hazard Assessment

The main concern with chemical A was that it is suspected of causing toxicity to reproduction. In other words, it would be considered a "particularly dangerous substance", see section 2.1. Chemical B is not believed to cause reproductive toxicity, but it has shown acute toxicity (ECHA, n.d.-b). The toxicity to reproduction of chemical A and B has been assessed through studies on rats (ECHA, n.d.-c), using OECD guideline tests (more about these types of tests in the background section, see 2.6.1.1). Exposure to chemical A to the pregnant rat caused abnormalities in the offspring that could lead to the offspring dying (ECHA, n.d.-c). While effects on post implantation loss of the foetus could be seen in the case of chemical B, these effects were not believed to be linked to reproductive toxicity but due to other effects caused in the maternal rat. Hence it was not classified as a reproductive toxicant.

4.1.1.1 PBT Assessment

As neither chemical A nor B fulfils the criteria for persistence or bioaccumulation, they are not classified as PBT (nor vPvB) substances. They are not persistent since they are both readily biodegradable and are not expected to bioaccumulate (ECHA, n.d.-c). Chemical B does not meet the criteria for toxicity either. Since chemical A is classified as toxic to reproduction (category 1B), it fulfils the criteria for toxicity, but a substance would need to fulfil all the criteria for persistence, bioaccumulation as well as toxicity in order to be classified as a PBT substance.

4.1.1.2. No Effect Levels for Ecotoxicity and Human Toxicity

Tables 4.1 and 4.2 below presents the toxicological summaries for DNELs and PNECs for chemical A and B, respectively (ECHA, n.d.-c; AkzoNobel, 2013; AkzoNobel, 2017). As can be seen, chemical B has in most cases higher threshold values than chemical A, due to the low no effect levels for chemical A based on reprotoxic effects. The exception is sewage treatment plant (STP) where chemical B has a relatively low PNEC due to inhibition of respiration of nitrifying bacteria. Chemical B could potentially be expected to have lower acute DNELs than chemical A. For example, this can be seen for systemic effects from acute inhalation exposure. For more detailed tables that include most sensitive endpoints, see section 8.1 in appendix.

Table 4.1 Toxicological summary with DNELs for chemical A and B, for general population (consumers) and workers.

Hazard via…			**DNEL (general population)**		**DNEL (workers)**	
			Chemical A	**Chemical B**	**Chemical A**	**Chemical B**
Inhalation	Long term	Systemic	0.2 mg/m^3	5 mg/m^3	0.7 mg/m^3	20 mg/m^3
		Local	n/a	Exposure based waiving	Medium hazard	0.9 mg/m^3
	Acute/ short term	Systemic	No hazard identified	30 mg/m^3	No hazard identified	90 mg/m^3
		Local	n/a	Exposure based waiving	Medium hazard	3 mg/m^3
Dermal	Long term	Systemic	1 mg/kg bw/day	5 mg/kg bw/day	2 mg/kg bw/day	10 mg/kg bw/day
		Local	20 µg/cm^2	Exposure based waiving	30 µg/cm^2	1000 µg/cm^2
	Acute/ short term	Systemic	n/a	5 mg/kg bw/day	No hazard identified	Exposure based waiving
		Local	n/a	Exposure based waiving	Medium hazard	Exposure based waiving
Oral	Long term	Systemic	0.1 mg/kg bw/day	n/a	n/a	n/a
		Local	1 mg/kg bw/day	n/a	n/a	n/a
	Acute/ short term	Systemic	n/a	Exposure based waiving	n/a	n/a
		Local	n/a	n/a	n/a	n/a
Eyes		Local	n/a	No hazard identified	High hazard	No hazard identified

* n/a = Information about DNEL not available in REACH registration dossier.
** Exposure based waiving = exposure is believed to be limited.

Table 4.2 Ecotoxicological summary with PNECs for chemical A and B.

Hazard for...		**PNEC**	
		Chemical A	**Chemical B**
Aquatic organisms	*Freshwater*	0.02 mg/L	0.6 mg/L
	Marine water	0.002 mg/L	0.06 mg/L
	STP	80 mg/L	6 mg/L
	Sediment (freshwater)	0.2 mg/kg sediment dw	1000 mg/kg sediment dw
	Sediment (marine water)	0.02 mg/kg sediment dw	100 mg/kg sediment dw
Air		No hazard identified	No hazard identified
Terrestrial organisms	*Soil*	0.02 mg/kg soil dw	8 mg/kg soil dw
Predators	*Secondary poisoning*	1 mg/kg food*	No potential for bioaccumulation

* = Note, that while the previous RA on chemical A (AkzoNobel, 2013) did not include PNEC for secondary poisoning for chemical A, based on no potential for bioaccumulation, there was a PNEC for this available in the REACH dossier.

As mentioned in the method section, the DNELs used in this study were based on the DNELs from the previous RA and CSR on chemical A and B done on behalf of AkzoNobel, and DNELs available in the REACH registration dossier on ECHA's website. While the DNELs used in this RA were the same as was previously used for chemical B in the CSR by AkzoNobel, there are some difference for the DNELs used for chemical A. The difference is the dermal DNELs for long-term systemic effects, which are about 10 times smaller than the ones previously used in the RA by AkzoNobel. The reason for this was that the DNEL calculations were updated by AkzoNobel after the RA on chemical A. This was due to uncertainties surrounding the no effect levels of the toxicity to reproduction for chemical A, and to account for this a BMD was used as point of departure.

It can also be noted that there are many exposure routes for which no DNEL is derived. However, as mentioned before, the focus of this RA was the systemic effects from long term exposure (to capture potential risks of toxicity to reproduction), and as can be seen the only

DNEL then missing was for oral exposure to chemical B. This exposure was instead assessed using a qualitative risk characterisation, see section 4.1.3.2.

The PNECs were the same as previous RA for chemical A for freshwater, marine water and STP, whereas the sediment and soil PNECs in the REACH dossier (used in the table above) were about 10 times smaller. For chemical B, the PNECs available in the REACH dossier were the same as previously used in the CSR.

4.1.2 Exposure Assessment

4.1.2.1 Workers

The resulting calculated exposure is presented in table 4.3, divided into each process and intervals for the exposures from the different PROCs used to describe the activities therein. As mentioned previously, these are also the same exposures that was calculated in the previous RA for chemical A (AkzoNobel, 2013).

Table 4.3 Exposures to workers, calculated in ECETOC TRA.

		Long-term Inhalative Exposure Estimate (ppm for volatiles)*	Long-term Inhalative Exposure Estimate (mg/m^3)*	Long-term Dermal Exposure Estimate (mg/kg/day)	Short-term Inhalative Exposure Estimate (mg/m^3)	Local Dermal Exposure Estimate ($\mu g/cm^2$)
Manufacturing of chemical A and B *and* **Production of softener**	*Chemical A*	0.01-0.15	0.043-0.65	0.034-0.27	0.17-2.6	10-20
	Chemical B	0.01-0.15	0.043-0.64	0.034-0.27	0.17-2.6	10-20
Use of softener in textile wet treatment	*Chemical A*	0.10-0.15	0.43-0.65	0.14-0.27	1.7-2.6	20
	Chemical B	0.10-0.15	0.43-0.64	0.14-0.27	1.7-2.6	20

* = The two types of inhalative exposures are the same amount but expressed with different units.

The exposure ranges (from lowest exposure to highest) is the same for manufacturing of chemical A and B, and the production of the softeners. The use of softener in textile wet treatment generates almost the same exposure intervals, but the lowest exposure is higher than for the other two processes. As can be seen, the difference in exposure to chemical A and B is very small. What differs is the inhalation exposure, and this small difference is due to the difference in molecular weight. The difference in vapour pressure between the chemical was not reflected in the exposure results as both chemicals were categorised as low fugacity chemicals. It should also be noted that these exposures were calculated with vapour pressures for chemical A and B at 20°C. The vapour pressures are not extrapolated by ECETOC to be valid for other temperatures. Hence, depending on the process temperatures, the inhalative exposures could be higher than these derived ones in warm processes. A sensitivity analysis of the chemical properties in ECETOC can be found in the following section.

4.1.2.1.1 Sensitivity Analysis

The effect of chemical properties input parameters on the resulting exposures were assessed by changing each property ± 50% (for biodegradability it was instead changed from readily biodegradable to not biodegradable). The following sensitivity analysis was done on chemical A, for PROC 6 as one of the activities in the use of softener in textile wet treatment.

Table 4.4 Sensitivity analysis results on chemical A.

		Difference in exposure compared to base setting				
Property	**Change**	**Long-term inhalative exposure (ppm)**	**Long-term inhalative exposure (mg/m^3)**	**Long-term Dermal Exposure (mg/kg bw/day)**	**Short-term Inhalative Exposure (mg/m^3)**	**Local Dermal Exposure ($\mu g/cm^2$)**
Molecular weight (g/mol)	*- 50%*	0%	- 50%	0%	- 50%	0%
	+ 50%	0%	+ 50%	0%	+ 50%	0%
Vapour pressure (Pa)	*- 50%*	0%	0%	0%	0%	0%
	+ 50%	0%	0%	0%	0%	0%
Water solubility (mg/L)	*- 50%*	0%	0%	0%	0%	0%
	+ 50%	0%	0%	0%	0%	0%
Partition coefficient (Kow)	*- 50%*	0%	0%	0%	0%	0%
	+ 50%	0%	0%	0%	0%	0%
Biodegradability test result	*Not biodegradable*	0%	0%	0%	0%	0%

As can be seen, the only change that impacted the result was the molecular weight. These results indicate that ECETOC use wide intervals for all of the chemical properties, not only for the vapour pressure as mentioned in 3.2.4.1. In other words, it does not reflect a difference in exposure due to different chemical properties unless the difference between the properties is big enough for the next interval to be used. This could therefore result in both under- and overestimates of exposure (and hence risk) for workers.

4.1.2.2 Consumer

Table 4.5 below presents the calculated amount and exposure to chemical A/B, based on the assumptions and calculations presented in the method. For these exposures, dipping method was used with a dose of 8 g softener/kg fabric, on both yarn, fabric and garment.

Table 4.5 Calculated exposure to consumers, for different exposure routes, and related amounts (based on dipping using 8 g softener/kg fabric).

Total softener added to textile wet treatment	24 g/kg textile
Softener in final garment	12 g/kg textile (1.2%)
Chemical A/B in garment	0.12 mg/kg textile (0.12 ppm)
Daily exposure to consumer through wearing garment	0.0096 mg
Daily oral exposure to children	0.12 mg
Air concentration of chemical A/B from garment	0.060 mg/m^3 (air volume: 2m^3)
Local dermal exposure through wearing garment	0.000006 mg/cm^2

4.1.2.3 Environment

In table 4.6 below, the result from the exposure assessment that relates to environmental exposure are presented. As can be seen, this focused on emissions to water.

Table 4.6 Calculated exposures and amounts related to environmental exposures (based on dipping using 8 g softener/kg fabric).

Amount of water used in textile wet treatment	24 L/kg textile
Amount of wastewater from textile wet treatment	12 L/kg textile
Softener in wastewater	1 g/L
Chemical A/B in wastewater from textile wet treatment	0.01 mg/L
Chemical A/B in freshwater (textile wet treatment)	0.001 mg/L
Chemical A/B in marine water (textile wet treatment)	0.0001 mg/L
Chemical A/B in wastewater from washing machine (residential washing)	0.019 mg/L
Chemical A/B in freshwater (residential washing)	0.0019 mg/L
Chemical A/B in marine water (residential washing)	0.00019 mg/L

4.1.3 Risk Characterisation

The calculated RCRs will be presented in the following sections.

4.1.3.1 Workers

The highest risk characterisation ratios for systemic effects from long-term exposure is presented in table 4.7 below. The rest of the RCRs for all PROCs and exposure routes can be found in the appendix (section 8.3).

Table 4.7 Calculated RCRs for workers.

	Risk Characterisation Ratios						**Legend:**
	Manufacturing of chemical A and B		**Production of softener**		**Use of softener**		**RCR < 0.5**
	Chemical A	*Chemical B*	*Chemical A*	*Chemical B*	*Chemical A*	*Chemical B*	**0.5 ≤ RCR < 0.75**
Inhalation	0.9	0.04	0.9	0.04	0.9	0.04	**0.75 ≤ RCR < 1**
Dermal	0.1	0.02	0.2	0.02	0.1	0.02	**RCR ≥ 1**

As can be seen, all risk characterisation ratios are below 1 and hence, there are no uncontrolled risks according to this result. While all the calculated RCRs are below 1, some of the PROCs (see appendix) have RCRs very close to 1. Keep in mind that the exposures are calculated based on assumptions of different personal protection equipment, and that the sensitivity analysis on chemical properties in ECETOC indicated that this tool can give a very rough estimate of exposure (see section 4.1.2.1.1), which can result in both underestimation or overestimation of risks.

4.1.3.2 Consumer

In the table below are the risk characterisation ratios for consumers presented. As can be seen, all RCRs are low and there are no risks shown from these calculations. The RCRs are very low for both chemicals. The dermal RCRs were calculated based on a leachable fraction of 10% in the exposure assessment, and even without leachable fraction the RCR would still be very low.

Table 4.8 Calculated RCRs for consumers.

	Risk Characterisation Ratios		**Legend:**
	Chemical A	*Chemical B*	
Dermal exposure to women	0.0002	0.00003	
Local dermal exposure to women	0.0004	*	**RCR < 0.5**
Inhalation by women	0.3	0.01	**0.5 ≤ RCR < 0.75**
Dermal exposure to children	0.002	0.0004	**0.75 ≤ RCR < 1**
Oral exposure to children	0.3	< 0.3	**RCR ≥ 1**

* = No RCR for local dermal exposure for chemical B due to no DNEL available (see table 4.1).

4.1.3.3 Environment

The calculated RCRs for aquatic toxicity is presented in table 4.9 below.

Table 4.9 Calculated RCRs for aquatic organisms.

	Risk Characterisation Ratios		**Legend:**
	Chemical A	*Chemical B*	
Freshwater (textile wet treatment)	0.05	0.002	**RCR < 0.5**
Marine water (textile wet treatment)	0.05	0.002	**0.5 ≤ RCR < 0.75**
Freshwater (residential washing)	0.09	0.004	**0.75 ≤ RCR < 1**
Marine water (residential washing)	0.1	0.004	**RCR ≥ 1**

4.1.3.4 Robustness Assessment

Table 4.10 below shows the calculated required amount for a risk to occur. As mentioned in the method, this was based on long-term systemic effects from chemical A on women, and oral exposure to children. The required exposures are on a daily basis.

Table 4.10 Scale of exposures that would give uncontrolled risk for consumers.

	Required amount (for RCR=1)
Chemical A residues in fabric	640 mg/kg textile
Chemical A residues in softener	6.7 %
Softener in fabric	80 kg/kg textile
Textile products (dermal contact)	5300 kg
Textile products (inhalation)	2.9 kg (2 m^3) 29 kg (20 m^3)
Drinking water (wastewater from textile wet treatment)	640 L
Textile products (oral exposure to children)	3.8 kg

The required chemical A residues in fabric were based on the leachable fraction of 10% but does not account for any skin-factor. The required chemical A residues in softener, or the amount of softener that is required to be in the fabric, are then based on this residue level.

For textile amount required for risk through dermal contact, this is not realistic when keeping in mind that this would be the required quantity of textiles to be exposed to during the course of one day. Neither is the amount of water. For inhalation, which arrived at values closest to realistic amounts, it should be remembered that these numbers were based on worst-case assumptions (as is the case with the other amounts as well). All of these required amounts are also significantly increased if using the lower recommendation of softener (3 g/kg instead of 8 g/kg for dipping).

All the RCRs would exceed 1 for different exposure routes to the consumers, with 100% cleavage of the softener back into chemical A. For the environment, RCR for marine water would be >> 1 from both textile wet treatment and residential washing. These were based on the highest softener dose of 8 g/kg in dipping. At this point in time, we do not have the knowledge to estimate how likely the softener is to cleave back into chemical A and B, and so 100% cleavage was used as a worst-case scenario. Considering that cleavage above 100% would not be possible, and that the analysis done on the yarn currently being made by AkzoNobel have validated the amount of chemical A/B in the softener and fabric that was used in this RA (AkzoNobel, 2018, personal communication), it would also mean that if the softener is cleaving back into chemical A/B this would need to happen within the body or in the environment. Metabolic transformation within the human body of course requires that the softener itself is first absorbed by the skin from the garment. In the calculations assuming 100% cleavage, a leachable fraction of 10% have

been used. Whether or not the softener would leach out from the clothes to the same extent is not certain.

4.2 Life Cycle Assessment

4.2.1 Inventory Analysis

In this section, information about the inventory data for the softener life cycle is presented. The LCI part of this public report has been cleared of confidential information and the full LCI is presented in the confidential appendix.

4.2.1.1 Raw Material Production

Manufacture of chemical A and B is a multi-output process which produces several different chemicals. Production of chemical A and B are based on AkzoNobel's existing model in GaBi. As mentioned previously, direct emissions of chemical A and B from this process were not included and will hence be missing in the toxicity impact.

Due to confidentiality, information about the "other chemicals" that are used in softener production cannot be disclosed in this public report. Inventory for these chemicals were taken from Ecoinvent database. More detailed information about these are presented in the confidential appendix.

4.2.1.2 Softener Production

Chemical A and chemical B are transported to softener manufacturing plant as intermediate chemicals to produce softener A and B, respectively. A batch reactor is used in the model to mix the intermediate chemicals with the other chemicals used in the production of the softener. Different ratios of all raw materials are used to produce softener A and softener B. The water used for cleaning of the machinery that is used to produce the softener was assumed to be small and negligible, based on information from the softener producer.

4.2.1.3 Textile Wet Treatment

After softener production, the softener product is transported to the dye house plant which is also located in China. As mentioned earlier, this transport is however not included in the model. In this phase, other chemical substances are used such as reactive dyes, dyebath chemicals and other auxiliaries that are needed to give the colour to the fabric. However, these other chemicals were excluded from this LCA model, since this study focused only on the softener life cycle.

The inventory data for this process refers to softener being used to treat yarn, fabric and garment (these three processes were modelled as one process in GaBi and are based on a softener dose of 0.5% being used for dipping). This inventory data was collected from general data as mentioned in section 3.3.7, and from the calculations in the RA. Electricity to run the equipment was included and was based on jet dyeing machine as mentioned in section 3.3.8 (Roos et al., 2015b). The main difference between softener A and softener B in this step is in the dilution process. While softener A can be diluted using cold water, the dilution of softener B will need hot water. This difference can be seen in table 4.12 further below, where a heat source is needed for the

dyeing house using softener B. The heat used for softener B was based on heat used in jet dyeing machine (Roos et al., 2015b), due to data gap for the actual heating required. The water used in this step (see section 3.1.2) was included in the inventory but excluded from the model.

4.2.1.4 Use Phase

The finished garment is then transported to retailer and thereafter used by consumer. It was assumed that in residential washing, 20% of the softener is washed out in every washing and based on the public data by Roos et al. (2015b) the number of washes during 1 year is 11 times, according to T-shirt life time. From the calculation, the amount of softener that stayed in the fabric until the end-of-life was 9% of the total softener.

The energy and water use from washing the garment was allocated to the garment and not the softener and was consequently excluded from the model. It was assumed that 100% of chemical A and B in the garment washed out during this 1 year. Like for the other processes, WWTP was only included in terms of biodegradation of these direct emissions being accounted for.

4.2.1.5 End-of-Life

In the end-of-life phase, residues of softener in the fabric (9% of the total softener on the garment, as mentioned in section 4.2.1.4) was assumed to be incinerated together with the fabric in the municipal solid waste (the general emissions from this process was allocated only based on the amount of softener in the fabric, while the impact from the fabric was not included). The data for the incineration was based on an Ecoinvent process, which is "disposal, municipal solid waste, 22.9% water, to municipal incineration".

4.2.1.6 Incineration of Chemical A and Production of Alternative Fuel

One of the alternative future uses in this case study was to bring chemical A to an incineration plant, where it would be combusted and together with the waste converted into ash, flue gas and heat. However, due the fact that there is no incineration plant at the current plant in China, the inventory data for this process was gathered from AkzoNobel's database in Sweden. The alternative types of fuel that was compared in this study was wind and coal.

4.2.1.7 Characterisation Factor for Toxicity

Based on data from the RA the characterisation factors for human toxicity impact was calculated, while characterisation factors for ecotoxity was already available in the USEtox model. Both types of characterisation factors are presented in the table below.

Table 4.11 Characterisation factor for toxicity impact.

	Characterisation factors for Ecotoxicity (PAF.m^3.day/ kg emitted)		**Characterisation factors for Human Toxicity (cases/kg emitted)**	
	Emission to Air	*Emission to Fresh Water*	*Emission to Air*	*Emission to Fresh Water*
Chemical A	< 1.5	< 90	4E-07	5E-07
Chemical B	> 1.5	> 90	10E-08	2E-07

* PAF = Potentially Affected Fraction

4.2.1.8 Aggregated Inventories for Scenario 1 and 2

Table 4.12 presents an aggregated inventory of some of the involved processes in scenario 1 and 2. The full inventory cannot be disclosed due to confidentiality. This inventory starts from the textile wet treatment and includes the other downstream processes, while the processes upstream from textile wet treatment (such as softener manufacturing) are not included in the table (but are included in the model). As mentioned in the previous sections, these processes were modelled using process data from Ecoinvent and AkzoNobel. Outputs in the table are limited to emissions of chemical A and B, and the generated heat used for energy recovery (the model itself includes more outputs).

Table 4.12 Aggregated inventory of downstream processes in the system for the different scenarios.

			Scenario 1	**Scenario 2**	
IN	**Softener**		1	-	kg A
			1	2	kg B
	Electricity		2.48	2.48	MJ
	Heat		4.47	8.93	MJ
OUT	**Emissions to water**	**Chemical A**	9.75E-07	-	kg
		Chemical B	8.35E-07	1.67E-06	kg
	Emissions to air	**Chemical A**	2.50E-06	-	kg
		Chemical B	2.50E-06	5.00E-06	kg
	Energy*		-	2.04	MJ

* = Energy generated from incinerating chemical A and used for energy recovery in scenario 2.2 and 2.3 to replace coal and wind, respectively.

4.2.2. Impact Assessment

In this section, the result from scenario 1 and 2 are presented and explained. The objective of this case study was to answer which option is preferable: continued or discontinued use of chemical A. This part also includes a closer analysis of the hotspots and what details that causes the difference in the overall life cycle of softener A and B. Since most of the results from the different impact categories showed a similar trend (see appendix 8.4), the discussion is focused on climate change and non-cancer toxicity.

4.2.2.1 Scenario 1

In the first scenario, environmental impacts from parallel use of both softeners were modelled. Total impact (in terms of climate change potential) for the scenario 1 is presented in figure 4.1. The result indicates that softener B gives a slightly higher impact than softener A, but the climate change impacts from the two softeners are almost identical. Comparing the kg CO_2-equivalents from the life cycle of softener B with softener A, it can be seen that softener B is approximately 6% higher than softener A. It is worth to look into details to identify the hotspots of CO_2-equivalents emission. It can be seen that climate change impact for the whole softener life cycles are mainly driven by the production stage.

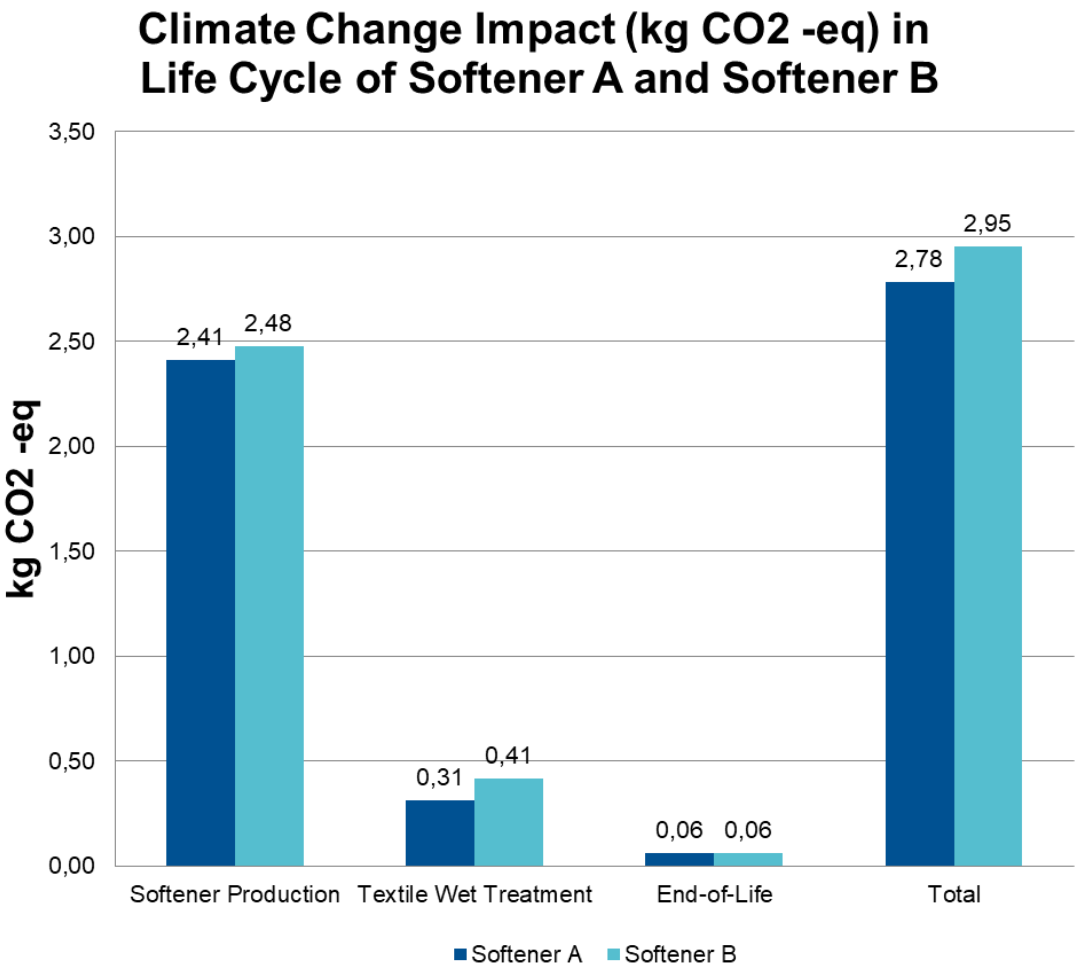

Figure 4.1 Climate change impact in life cycle of softener A and softener B. The softener production includes production of the raw materials.

Based on figure 4.1 it could also be seen that use of softener in the wet treatment appears to be the main reason for the difference between softener A and softener B. This difference is because the dilution process of softener B involves heating of hot water, as mentioned in the inventory analysis. As also mentioned previously, impacts related to the water used in textile wet treatment was not included in the model (besides this additional heating that softener B dilution requires). For the end-of-life (municipal incineration), the climate change impact was calculated based on the mass of softener incinerated (by incinerating garment).

The production of softener A and B involves the mixing of different raw materials. The impact from these raw materials (aggregated due to confidentiality) on softener production is presented in figure 4.2. It can be seen that in the softener manufacturing, production of other raw materials contributes to higher impact than production of chemical A/B, electricity, heat or transportation of (all) raw materials.

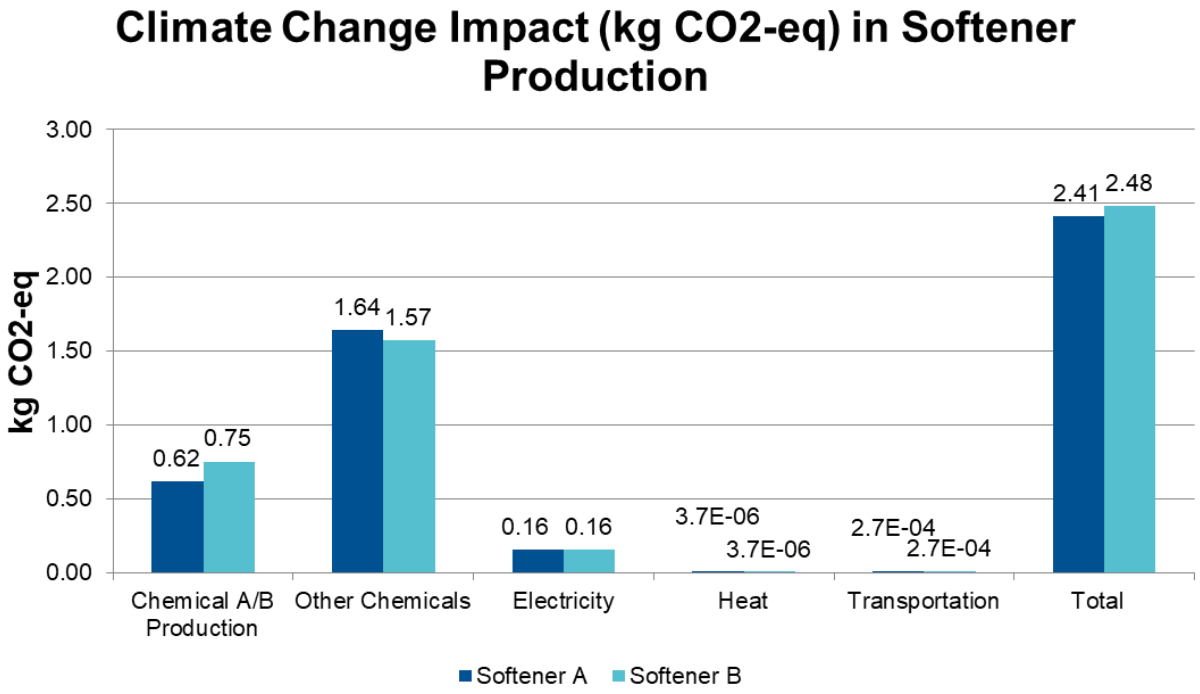

Figure 4.2 Climate change impact in softener production.

4.2.2.2 Scenario 2

In scenario 2, chemical A was incinerated, and chemical B production was increased in order to fulfil the FU by substitution of softener A. In figure 4.3, the impact of scenario 1 is compared to scenario 2, with its different options: with and without energy recovery and the different types of alternative fuels to produce the (replaced) electricity. The amount of chemical A in the chemicals

production was increasing corresponding to the increasing need of chemical B to produce 2 kg softener B. The impact from the production of chemical A is also included in the graph.

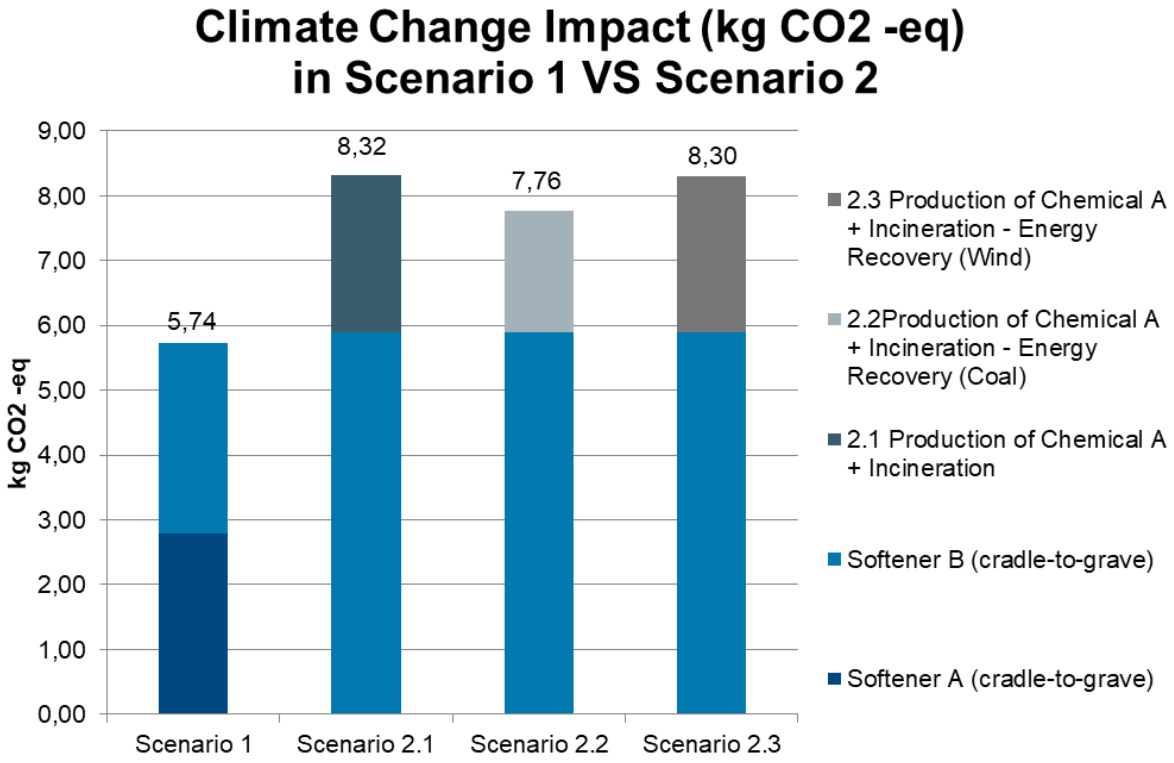

Figure 4.3 Climate change impact in scenario 1 compared to scenario 2.

From the comparison of these scenarios, it can be concluded that the discontinued use of softener A would bring higher climate burden. This is due to the fact that the use of twice the amount of softener B will contribute to more climate change impact than the parallel use of softener A and softener B. Three different options for incineration are presented and as seen in the graph above, incinerating chemical A without recovering the energy (scenario 2.1) will be the option with the highest potential climate impact, with 8.32 kg CO_2-eq per functional unit. For the options with energy recovery, replacing energy based on coal contributes to a slightly lower impact than replacing energy from wind. This difference is due to the fact that producing energy from coal contributes to a higher level of CO_2-eq emissions than wind. Replacing a certain amount of energy from coal therefore means that a greater amount of emissions is replaced, which lowers the total impact of the system to a greater extent compared to replacing energy produced with lower impact (such as wind power). In figure 4.3, it can also be seen that even though the energy from the incineration process is used to replace the energy need in the plant, the environmental burden is still higher than the first scenario.

4.2.2.3 Toxicity Impact

The characterisation factors calculated in the USEtox model was added to GaBi to calculate human toxicity impact. The results for this impact (non-cancer) for scenario 1 is presented in figures 4.4, and figure 4.5 compares this result with scenario 2.

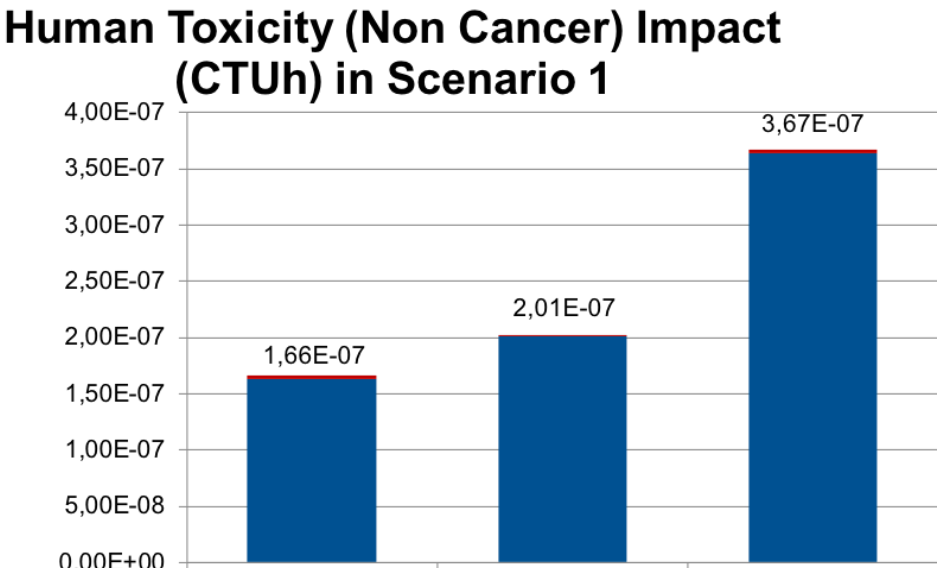

Figure 4.4 Human toxicity impact in scenario 1.

The graph above represents the human toxicity impact from direct and indirect emission. Direct emissions refer to emissions of chemical A and chemical B, and indirect emissions are other chemicals emitted from different activities in the life cycle. It can be seen from the bars that direct emissions from softener A life cycle is higher than for softener B. However, softener B contributes to a higher impact to human toxicity from indirect emissions.

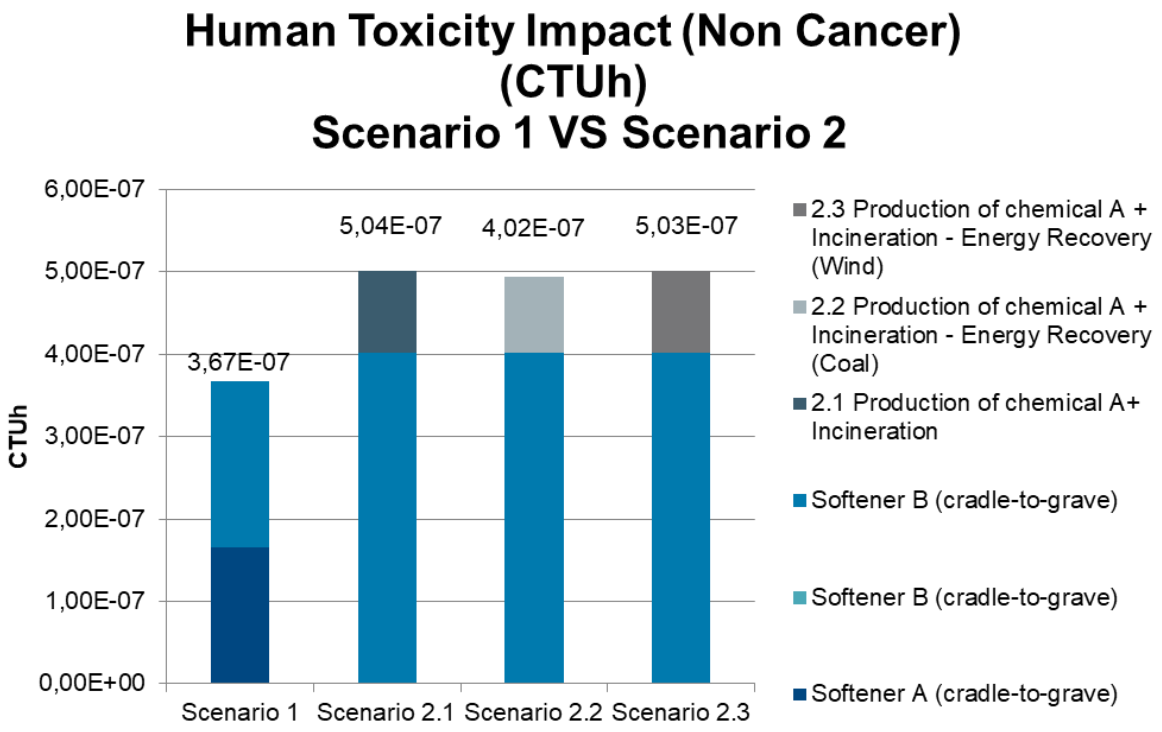

Figure 4.5 Human toxicity impact in scenario 1 compared to scenario 2.

For the comparison between scenario 1 and scenario 2, seen in figure 4.5 above, it is clear that human toxicity impact potential in scenario 1 is lower than scenario 2 (for all three different options). Since the impact from softener A is lower than softener B (as seen in figure 4.4), doubled use of softener B will result in higher impact for human toxicity.

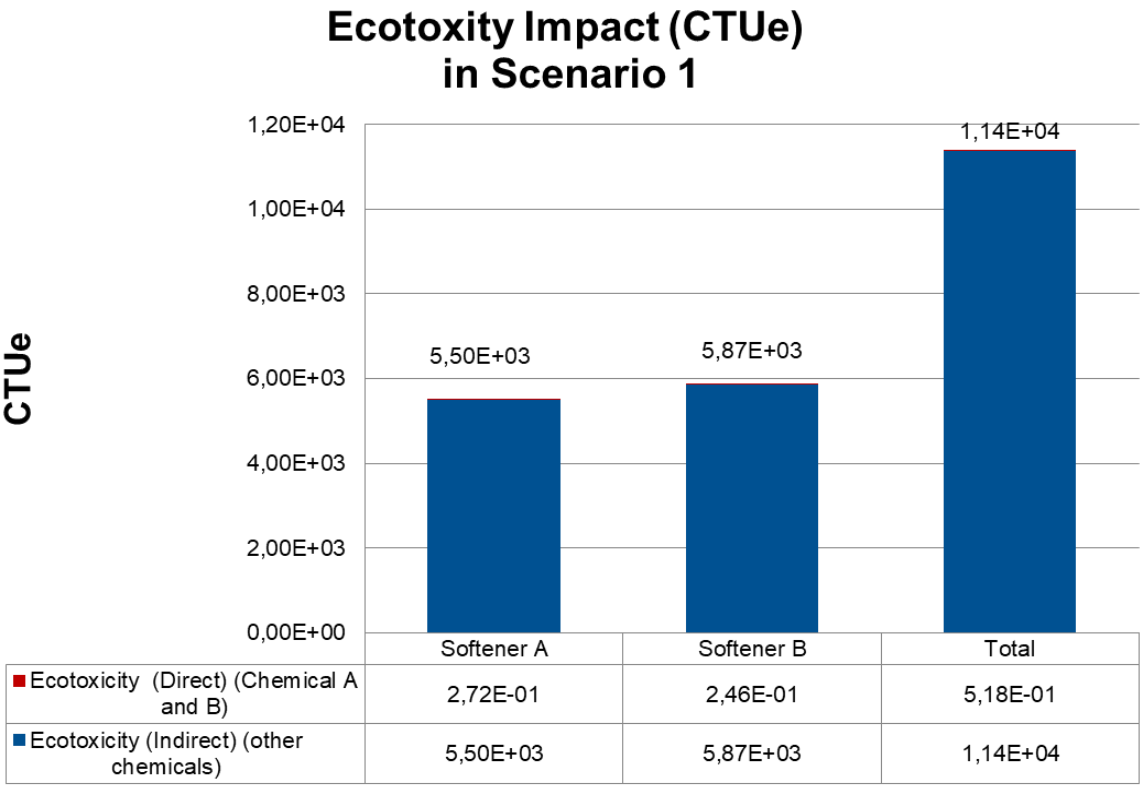

Figure 4.6 Ecotoxicity impact in scenario 1.

Based on figure 4.6, the ecotoxicity from softener A and softener B was compared. The result shows that ecotoxicity impact from softener B is only slightly higher than softener A. It should be noted here that most of the ecotoxicity impact comes from the indirect emissions of other chemicals from different activities, and not from direct emissions of chemical A and B. For the comparison of scenario 1 and 2 (figure 4.7), it can be seen that most of the ecotoxicity impact are from the main parts of the softener life cycle, while the incineration processes give a small impact in comparison. The reason behind this is further explained in the discussion section.

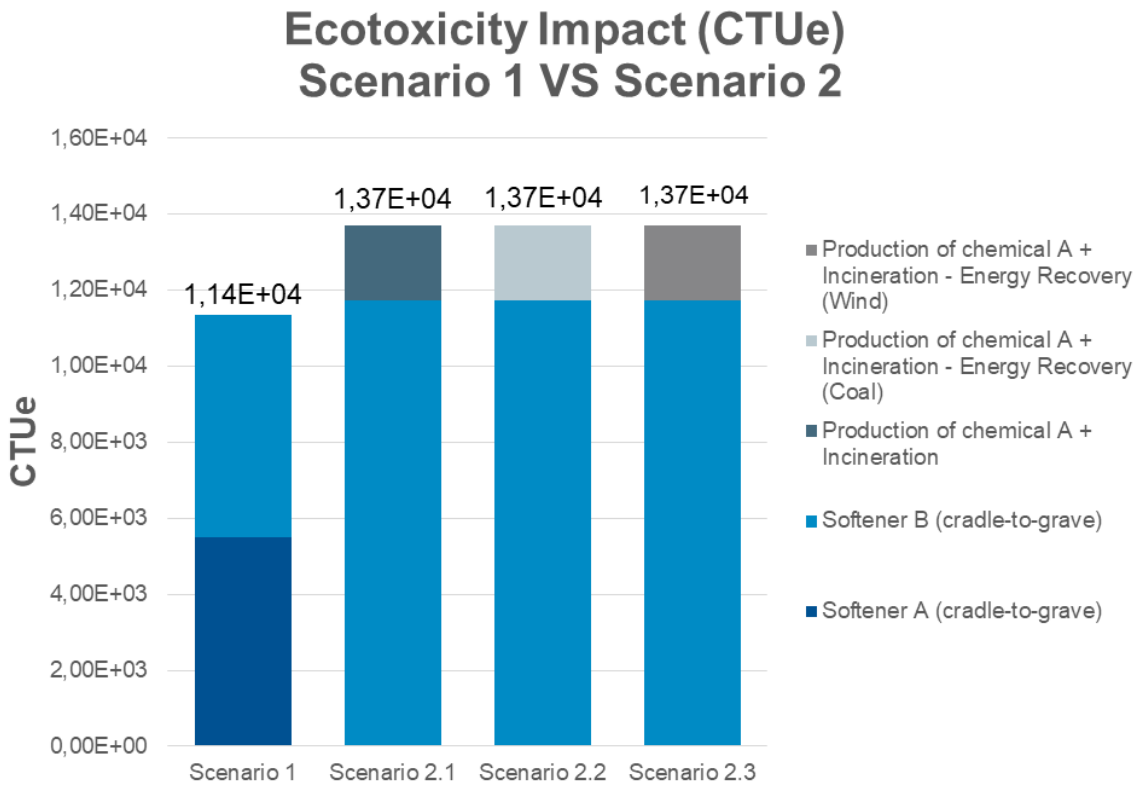

Figure 4.7 Ecotoxicity impact in scenario 1 compared to scenario 2.

4.2.2.4 DALY in Life Cycle Assessment

In this case study, climate change, ozone depletion and human toxicity (cancer and non-cancer) impact potentials were converted to effects on human health, expressed with DALYs. As mentioned earlier, DALY can be calculated with conversion factors using ReCiPe and USEtox methods for different impact categories. The resulting DALYs can be seen in table 4.13 and 4.14 below.

Table 4.13 DALY results from LCA for Scenario 1 (years per kg softener).

	DALY	
	Softener A	*Softener B*
Global Warming - Human health	2.6E-06	2.7E-06
Stratospheric ozone depletion - Human health	3.2E-11	6.1E-11
Human Toxicity (cancer)	2.0E-07	2.1E-07
Human Toxicity (non-cancer)	1.9E-06	2.3E-06
Total DALYs	4.7E-06	5.3E-06

Table 4.14 DALY Results for Scenario 1 VS Scenario 2 (years per functional unit (2 kg softener)).

	DALY			
	Scenario 1	*Scenario 2.2*	*Scenario 2.2*	*Scenario 2.3*
Global Warming - Human health	5.3E-06	7.7E-06	7.2E-06	7.7E-06
Stratospheric ozone depletion - Human health	9.2E-11	1.3E-10	1.3E-10	1.3E-10
Human Toxicity (cancer)	4.1E-07	5.2E-07	5.2E-07	5.2E-07
Human Toxicity (non-cancer)	4.2E-06	5.8E-06	5.7E-06	5.8E-06
Total DALYs	1.0E-05	1.4E-05	1.3E-05	1.4E-05

5. Discussion

5.1 Risk Assessment

5.1.1 Workers

In this RA, there were no RCRs equal to or higher than 1, however for some of the PROCs for workers the RCRs were very close to 1. This was the case for both chemical A and B. For chemical A, the RCRs close to 1 were for long-term exposure, whereas for chemical B it was short-term exposure. These results are of course dependent on the assumptions made regarding activities within the processes and the level of personal protection equipment used during these. As mentioned, the selection of PROCs were based on previous work done by AkzoNobel. It should however be noted that the information acquired about the downstream processes (softener production and dye house) were somewhat limited. We hence recommend that for future studies, further communication with the softener producer, as well as the dyeing house, should be made in relation to this - to ensure that the activities (PROCs) and personal protection equipment that are modelled correctly reflects the true situation. Based on our RCRs, we recommend that the level of personal protection equipment used by workers should be increased (to get a higher safety margin to RCR=1, especially to protect the most sensitive group, i.e. women in fertile age). Again, it should be noted that the assumptions used in our calculations could have resulted in an overestimated exposure.

In the calculated exposure to workers, there was only a very small difference between chemical A and B. In the sensitivity analysis made on chemical properties input parameters in ECETOC, it became evident that the result is not very sensitive to the properties of chemicals, and that the difference in exposure between chemical A and B were due to a (small) difference in molecular weight (with equal exposure on a molar basis) and not from the rather big difference in vapour pressure as could be expected. There were also other indications that it can be hard to make a site-specific exposure estimation using ECETOC. When modelling worker exposure in ECETOC, the amount of product used is not one of the input parameters but instead, the level of the certain chemical is chosen. The problem is that these are in very rough intervals (to choose from in the ECETOC model file), with the lowest option being <1% and the highest >25%. As the residues of chemical A and chemical B in the softener were assumed to be 0.001% (10 ppm), using concentrations to potentially up to 1% in the calculations could result in a significantly higher exposure. This would then lead to an overestimation of the risks to workers, and as previously mentioned, some of the RCRs were very close to 1. A sensitivity analysis on the personal protection equipment and other parameters available in ECETOC could also be done to assess the sensitivity of the results from this tool. To do a more site-specific exposure assessment of workers should preferably be the focus in future studies, to further ensure that there truly is safe use of the chemicals in industrial sites. It should be looked into if more accurate exposures can be calculated, maybe using a tool where differences in chemical properties are taken more into consideration. Future studies could also include the exposure to retailers, as they would be in contact with a great amount of new clothes.

As mentioned in the hazard assessment, there were exposure routes for which no DNEL was derived. This could potentially mean that there were uncontrolled risks that could not be seen in

this RA. For some exposures this was due to “exposure based waiving” or that toxicology studies has not indicated any hazard (hence no risk). “Exposure based waiving” means that the workers are assumed to not be exposed to high enough levels to give an effect, thanks to the safety equipment they wear or due to closed systems used in the process. While we did not calculate any DNELs ourselves in this RA, we recommened that for future studies DNELs should be calculated for the exposure routes where “exposure based waiving” previously has been used, as the conditions for exposures is highly dependent on the process design and personal protection equipment used, which can differ a lot between different types of applications, etc. (instead of a more general exposure based waiving as currently has been used).

5.1.2 Consumers

Based on our RA, there are no uncontrolled risks for consumers connected to chemical A and B being used in industrial fabric softeners. All assessed RCRs for consumers were very low for both chemicals, where chemical A showed higher values due to lower DNELs. For dermal contact, which was believed to be the main exposure pathway, the RCRs were smaller than 0.001. The highest RCRs were for inhalative exposure of women and oral exposure of children, and these were both based on significant worst-case assumptions. For example, for inhalation it was assumed that all chemical A in the fabric would evaporate (and roughly at the same time). It was also based on the assumption that nothing of these residues had already been absorbed through the skin. Even using these overestimated exposures, the RCRs for exposure were low. If taking both inhalation, dermal and oral (for children) exposure into account, the potential exposure through each exposure route would of course be even lower. For example, the higher amount of chemical A that evaporates from the clothes, the less residues will be left and available for the child to consume by putting the clothes in its mouth. As the RCRs using worst-case exposure were all below 1, more realistic scenarios like this were not done in this RA.

Controlled risks were also shown for exposure through drinking water, based on calculating backwards to the required amount of drinking water (equation 11), using worst-case assumptions. This was an overestimation, as in reality, the water not absorbed by the textile in textile wet treatment might be used again instead of being disposed of. And if and/or when disposed of, the wastewater would be diluted and wastewater treatment is likely to be in place. Since chemical A and B are readily biodegradable, the resulting levels after wastewater treatment would be very low/negligible. A more realistic exposure can of course be calculated, but as no risks were shown in our calculations this was not done in this RA.

The exposure to consumers through inhalation or oral uptake through dust containing textile fibres, released from the garment due to wear etc., was not assessed in this case study as it was assumed negligible in comparison to other exposure routes. For future studies that also include exposure to retailers (which was excluded from our study due to time constraints and data gaps), this could be a way of exposure that can be interesting to look into.

The RCRs for children were based on a DNEL for which the point of departure is correlated to toxicity to reproduction seen in the rat studies for chemical A. In these studies, the exposure to the maternal rat caused effects in the offspring. However, the direct exposure of offspring and possible effects were not studied. Therefore, it could be argued that whether or not these DNELs

accurately represent effects that could arise when children are exposed to chemical A is not known.

The animal studies on the reproductive toxicity of chemical A had shown some conflicting results in terms of LOAEL/NOAEL. The main uncertainty was that while one study had found a very low LOAEL, there were also effects seen in the control group, and hence it could not be confidently determined that the effects seen at the LOAEL were treatment related. This was due to lack of historical data on these particular effects. Due to this reason, as mentioned in the hazard assessment, a BMD was used as basis for the DNELs. Further animal studies focusing on these reprotoxic effects would hence be needed to determine a more certain no effect level and/or verify this BMD, understanding of the mode of action would also be of importance. Difference in no effect levels could have a significant impact on RCRs; especially when it comes to the workers, for which RCRs very close to one were seen. It would also be needed to get a more accurate assessment of human toxicity potential. But this would also be an ethical problem, in terms of animal rights. While *in vitro* studies could potentially be used to assess certain local effects, we suggest that *in vivo* studies are needed in order to assess the systemic effects. There is also, as always, uncertainty if the effects seen in these animals can be assumed to be the same in humans and what the corresponding no effect level for humans would be. While this is accounted for when applying assessment factors to derive DNELs, this is still something that can be important to keep in mind.

5.1.3 Environment

The RCRs for aquatic toxicity were low for both chemical A and B. As mentioned previously, the exposure to the environment was only assessed to a limited extent, using worst-case scenarios and assumptions for emissions to water (from textile wet treatment and residential washing of clothes). This was due to the limited time frame of the master thesis, since the main concern was the potential risks to the consumer this was the safeguard subject that was prioritised. Also considering the ready biodegradability of chemical A and B, environmental emissions were given lower priority as the exposure is likely to be very low if WWTP is in place. Furthermore, the previous RA by AkzoNobel on chemical A assessed environmental exposure by using ECETOC with different ERCs and showed no uncontrolled risks. In future studies, more site-specific assessment on environmental exposures could potentially be made, for which more contact with the downstream actors are needed. Emissions to the environment can also occur when the garment is incinerated or sent to landfill, if there are still residues of chemical A or B in the garment. While this was not assessed in this RA, it could potentially be interesting to assess in a future study. Since the softener is not believed to wash out as easily, there might be softener residues left and how these can interact and impact the environment should be analysed as well.

5.2 Life Cycle Assessment

5.2.1 Results in Scenario 1 and Scenario 2

The results from the LCA show that scenario 1 has lower impact than scenario 2 with its different options, both in terms of for example climate change impact and human toxicity impact, as well as aggregated results in the form of DALYs. Scenario 1 further show that softener A has

a slightly lower impact than softener B, approximately 6% lower. This difference is considered very small and can even be assumed to be negligible. Sensitivity analysis could be done to assess what impacts this difference.

In the softener production, the other chemicals indicated higher climate impact compared to chemical A and B. It is worth noting that the model built in GaBi for these other chemicals was based on global data, with different energy sources that might differ from current energy sources used in China. To achieve more site-specific results, actual data from the supplier of raw materials are needed. Our recommendation for the softener producer is to look into different alternative chemicals with lower environmental impact in order to reduce the impact from the other chemicals.

In the textile wet treatment, a WWTP process was first added to the model, to account for its contribution to climate change due to the energy requirement. The result then showed that the WWTP (from textile wet treatment) contributed to roughly around 10% of the climate change impact potential for the softener life cycle. However, including WWTP significantly impacted the result for ecotoxicity and human toxicity. The reason for this is while the input to the WWTPs in our model only consisted of chemical A/B and softener in the wastewater, including a WWTP in the model results in a general output from a WWTP. This output consists of a number of different chemicals, that has quite a significant impact on the indirect human and ecotoxicity (it became the main contributor to these impact categories). This is an allocation issue, as it can be discussed whether or not this general output belongs to our (softener) system. In our case, it was hence decided to not include a WWTP, as the energy requirement would be equal for the two softeners (if allocated based on amount of treated water, allocation based on total organic carbon (TOC) could give different impacts) whereas it could potentially distort the difference in toxicity impact. However, a WWTP effect on chemical A/B emissions was still included as biodegradation of chemical A and B was accounted for in the emissions from the processes, as mentioned in the method chapter.

Related to assumption on electricity used in textile wet treatment, it should be noted that the amount of electricity added in the GaBi model was taken from a dyeing process using jet dyeing machine, from a report by Roos et al. (2015). As mentioned in 3.3.8, this dyeing process was chosen since it included the use of softener in the inventory data. However, comparing the different process for dyeing in the report, it can be seen that the energy demand varies quite a bit, which means that the extrapolation done for our model has high uncertainties. Furthermore, while the results presented in this report are based on allocating this energy based on the amount of softener used in the process, another option could be to instead base it on amount of treated textile. The results based on textile allocation would give around 15 times higher amount of energy needed compared to allocation based on softener used. This would therefore give significantly higher result for the impacts related to energy. The heat needed in softener dilution was also allocated in the same way (based on amount of softener); hence, this could give an even higher impact for textile wet treatment if the heat was also based on amount of treated textile in this step.

Regarding the use phase and end-of-life phase, toxicity impacts were calculated based only on the emissions of chemical A and B, with the assumption that chemical A and B was 100% washed out when the consumer washes the garment (in the use phase). For the softener, the end-

of-life phase was based on the amount of softener left in the fabric once it was disposed of. With an assumption that 20% of the softener is washed out in each wash, 9% from total softener in the new garment was left after one year. As a result, the impact of incineration of softener was small compared to other phases. This might be an underestimation. Further information is needed to understand how much softener that stays in the fabric (until the end-of-life) and how much that ends up on the environment. More information about the properties of softener are also necessary to reduce uncertainties for the impact of these phases.

For the toxicity impact, the calculation of characterisation factors in the USEtox model was based on the data on no effect levels from the RA. However, as there are uncertainties regarding the no effect levels, especially for chemical A but also for chemical B as mentioned in the discussion on RA, this will increase the uncertainty for the characterisation factors. Our choice of no effect level as basis for characterisation factor for chemical A and chemical B can be an underestimation and overestimation of toxicity, respectively. However, the results for toxicity impacts, both for human and ecotoxicity, showed that indirect emissions were the dominant contributor compared to direct emissions of chemical A and chemical B. Hence, these choices of no effect levels should not have had a significant impact on the overall toxicity impact (and DALY) result. While the EFs from the ERCs used to estimate the direct emissions of chemical A and B are realistic worst-case, the total direct emissions can still be underestimated as emission from manufacturing of chemical A and B was not included in the model.

Regarding the direct ecotoxicity impact from chemical A and B, this was calculated using CFs that were already available in the USEtox model. As mentioned in section 2.5.3, there are uncertainties in the model that should be considered when interpreting the results. It should also be noted that there is a data gap due to air emissions being excluded from the calculation of ecotoxicity. For future studies, the air emission should be considered as it would have an impact on the ecotoxicity impact, in terms of that the contribution from direct emissions (chemical A and B) would be higher. However, while the air emissions (of chemical A and B) were between 20-30 times higher than the emissions to water (see table 4.12), the ecotoxicity CFs for air emissions were about 50 times smaller than the CFs for water emissions. This means that the impact this would have on total ecotoxicity impact should be limited. In order to make ecotoxicity impact more comparable with the RA environmental results, for future studies the ecotoxicity CFs can be calculated based on the same point of departures as the PNECs.

5.2.2 Uncertainties and Limitation

This LCA focused on the softener life cycle, so the production of textile was excluded in the studied system. However, the other chemicals and auxiliaries that are used in the textile life cycle, for example in wet treatment, might contribute to higher environmental impact and toxicity to humans. Inclusion of the textile would give a more straightforward A-LCA and give the possibility to relate softener related impacts with other impacts of the textile. While this current setting answers the question in our case, attributional LCA also including the life cycle of the textile can be done to get a better overview on how the impact from softener relates to the total impacts connected to the textiles. This could be used to find hot-spots of toxicity and other environmental impacts throughout the life cycle of softener.

Related to the impact from chemical A/B production, the model for this process has been built by AkzoNobel Sustainability team. Mass allocation was used to allocate the environmental impacts in this chemical production. It would be interesting to know how different the environmental impacts could be if this study was based on a different allocation method, since with mass allocation results in the chemicals with higher share of the in- or output from a process are given higher impact. Economic allocation for LCA of these chemicals could potentially result in rather different impacts. However, using economic allocation in the future scenario would be more complicated since the value of chemicals depends on current regulation.

From personal communication with the softener producer, transportation data for the other chemicals (used as raw materials in the softener production) was obtained. The transport related to other flows to and between processes were excluded. From the results (on softener production), it could be seen that the transport had very small impact compared to the other activities. Hence, the impact was considered to be negligible and other transportations in the life cycle were excluded from this study.

As mentioned in the method, due to the data limitation on textile wet treatment the heating required to dilute softener B was assumed to be the same amount of heat that is needed for a dyeing machine. This assumption might give underestimated results for the textile wet treatment. It also worth to know that the heating data from Roos et al. (2015b) was not directly to heat the water but mainly for heating the jet machine. The actual description and information from the dyeing house is needed to get more accurate heat and electricity data, and result; this is especially interesting as this is what is believed to be the main difference between the impact of the two softeners. Another limitation for this process was that the water use was not included in the model, as mentioned in section 3.3.6. Including this water would result in a significantly higher impact, for example climate change impact, for this process. Based on received information from the softener producer, the amount of water used would however be the same for softener A and B and including it should therefore not have had an impact on our overall result in comparing the two softeners and the different scenarios. However, for future studies, our recommendation is to include the amount of water used, which should be confirmed with the dye house. By adding water use in the model, the results seen in figure 4.1 would show higher impact than the current results with exclusion of water use.

It should be noted that for the direct emissions, the emission factors (EFs) for chemical A and B for softener life cycle are realistic worst-case EFs, and while it was assumed that there was emission abatement for emissions to water, the emission results might still be overestimated for this LCA study, since it was based on the choice for ERCs as well as data from the RA calculations (for how much softener that is absorbed by the fabric) which was also based on worst-case scenarios.

In scenario 2, it also should be noted that the data for incineration was based on AkzoNobel's incineration plant in Sweden, while currently there is no incineration plant built at AkzoNobel's plant in China. The energy production in the actual case might be different from Sweden's energy sources. The option of incineration without energy recovery can be seen as the most likely alternative if chemical A is instead sent to an incineration plant in another place, as a third-party waste management where recovery facility is not available.

It is important to note that the USEtox conversion factor from human toxicity to DALY is not chemical specific. This will of course add additional uncertainty, while also impact the implications of comparing these DALYs to ones potentially calculated from RA, since DALYs from RA would be chemical specific.

5.3 Combination of Risk Assessment and Life Cycle Assessment

As mentioned in the background (section 2.6.3), there are several different ways that are possible when it comes to the combination of LCA and RA. Based on the scope of this case study, our suggestion is to perform both LCA and RA separately to decrease the risk of potential problem shifting, if the result is used in decision making. Furthermore, these assessments should be performed based on methodological combinations in the following manner: performing a life cycle based risk assessment (LCBRA), that assesses potential risks throughout the life cycle of the chemicals, and inclusion of toxicological information about the chemicals in LCA by calculating (missing) characterisation factors with the help of the RA. Our suggestion on further aggregation or comparison of the result was to use DALYs. In our case, the RA showed no risks, and hence DALYs were only calculated for the LCA; which showed that scenario 1 gives slightly lower impact than scenario 2. As mentioned in the background, if DALYs are going to be calculated based on the RA as well, then they have to be based on the same assumptions as the LCA if a comparison is to be made. In order for DALYs to be calculated from the RA in our case, more information related to burden of diseases and actual cases would also be required. Otherwise a lot of assumptions would have to be made, as in RA risks are assessed on an individual basis, whereas LCA assess emissions and impact on a more generic basis for a population. However, as the RCRs in this RA were all below 1, it can be argued that the DALYs from the RA should be 0.

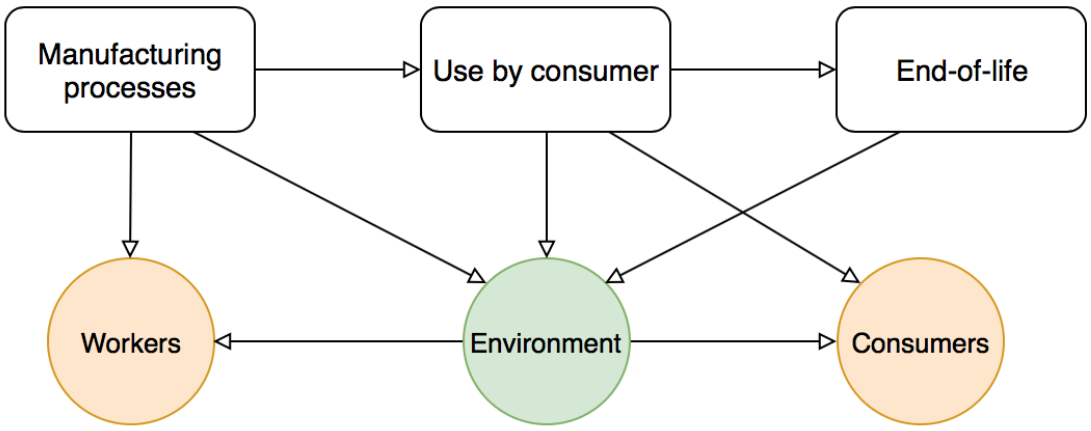

Figure 5.1 Type of exposure and risk to safeguard objects covered by the assessment tools in this study.

Figure 5.1 above is a representation of what types of exposures and risks that are covered in the LCA and RA for this case study. As can be seen, from the manufacturing processes (of chemical A/B, softener A/B and the garment (which includes textile wet treatment)) and use by consumer

(of the garment) there can be direct risks to workers and consumers, which were assessed using RA. The LCA then analysed the impacts from indirect risks (through emissions to environment). With this picture, we aim to show that since the LCA and RA in our case captures different aspects of the risks, the result from them can be added up (by using DALYs for example). In other cases, adding up the result from RA and LCA could result in double counting. The direct exposure to workers as well as consumers could potentially be captured with LCA. For example, using characterisation factors from USEtox for chemical A/B. To calculate the exposure to workers, the default emission factors (the ERCs) could be used (for example, to estimate direct emissions to air), but as mentioned previously (in the discussion on LCA), these might not be a good fit for the real scenario.

The DALYs now calculated for the LCA included calculating characterisation factors for chemical A and chemical B in USEtox. If DALYs were to be derived from both the LCA and RA, it would be important to base these on the same values (no effect levels) in order to make a comparison or add them up, as have been mentioned before. It is also important to not double count, and hence consider what type of exposures are accounted for in each assessment; an example would be if both DALYs includes emissions to water. Another thing to consider is that DALYs in LCA are usually calculated in relation to the functional unit. In order to make the DALYs comparable, the DALYs in RA also have to be calculated using the same basis. However, the DALYs calculated in risk assessments may not be easily related to the functional unit of LCAs. While setting the FU in LCA in a way that relates to the RA-exposure basis can be more straightforward, this can still be a challenge in the combination of the result from these two assessment tools.

The toxicity to reproduction tests done on chemical B did not lead to a classification of toxicity to reproduction, based on that the effects seen were believed to be caused by other means of maternal toxicity and not developmental toxicity. While we do not have the required knowledge to assess if this was a valid conclusion or not, our suggestion is that in future studies, the details of this animal study should be analysed in more detail, since it potentially can result in a significantly lower DNEL for chemical B. (In our case, there were no risks to the consumers, but this could have an impact on risks to workers.) Since adverse effects were in fact seen in this animal study, this NOAEL was used as a basis for the calculated DALYs for chemical B in the LCA, since it was lower than the NOAELs used as point of departure to the DNELs. This could be done as no DALYs were calculated from the RA (that would be added up or compared with DALYs from LCA), but if that were the case, the DNELs (used in the RA) and characterisation factors (for toxicity impact in the LCA) should be based on the same points of departure in order for the DALYs to be comparable. However, even if no DALYs were calculated for the RA, using a different point of departure for the DNELs and CFs still has implications on the overall result. Since a lower point of departure is used for chemical B in CF for LCA than in DNEL in RA, this means that the direct human toxicity impact is an overestimation compared to the RCRs in RA. Hence, the two results are not completely comparable. However, as can be seen in 4.2.2.3, the direct toxicity has very low impact on the total toxicity; therefore, the overall conclusion (scenario 1 vs 2) would not be impacted by changing to the point of departure now used. On the other hand however, changing the point of departure for chemical B DNELs would result in higher RCRs, which could mean uncontrolled risks for workers (based on the results using current assumptions).

For RA, DALYs could possibly be calculated utilising the benchmark dose curve to estimate the exposure. For this to be possible, more details about the benchmark study and access to the calculated curve would of course be needed. A tricky question with DALYs from RA is the type of effects that are expected. For example, if the effects would be a certain type of cancer, it is possible to look at statistics on how common this type is and use this in the derivation of the DALYs. However, it might not always be possible to find statistics like this, for instance in our case with toxicity to reproduction. If a risk would have been shown, the years lost due to early death would equal the full life expectancy for children, if following the effects seen to the offspring in some of the animal studies on rats. However, it can also be argued that years living with disability should also be taken into consideration for the parents, who would have lost these children. These aspects of DALYs do not have a straightforward solution.

The reason that we suggest doing both an LCA and RA, instead of doing only one form of methodological combination, is because this could omit important information about the whole system. For instance, if only performing an LCBRA, no information about climate change impact would be shown. This could then cause possible shifting of burden if used as sole decision basis. By only performing an LCA on the other hand, even if more toxicological information is included, the result would likely be for a general population, and not divided for workers and consumers (unless performing a very extensive LCA that includes exposure and impact on workers and consumers). It would hence not be as specific as an RA, and would not say anything about safety, from which can be concluded where risk management is most necessary.

A difference between LCA and RA in our case study is that while the RA calculates exposure based on two single chemicals, LCA takes the emission of several chemicals into consideration that is connected to the function of the product system. By performing a thorough attributional LCA, that incorporates as much toxicological information as possible on the chemicals involved, this would result in a more extensive view on the whole system. Then it would be easier to identify the different hot spots of environmental and toxicity impacts. For example, in regard to this case study, if the LCA would also include more data related to textile production and not just those related to softener production and use, it could be possible to see how the impacts to climate change, ecotoxicity and human toxicity (as well as the other impact categories) from softener compares to other chemicals used in other stages of the life cycle. An assessment like this would however be very time consuming and a lot of data would be needed.

An even more important difference is that the RA was based on several worst-case assumptions, as a way to handle uncertainty in data. If no risks are shown in a worst-case scenario, one can with more certainty say that there should be no risk in the real scenario. However, the LCA was not based on worst-case assumptions to the same extent, since the LCA is supposed to reflect the impacts from a more realistic scenario. This is something that is important to consider when comparing results from these two assessment tools. While we only calculated DALYs from the LCA, if DALYs were also to be calculated from the RA, it might therefore not be possible to just add them up.

5.4 Management of Hazardous Chemicals in a Circular Economy

The frameworks of circular economy and non-toxic environment do not always agree. The main idea with circular economy is to create circular flows, in which materials are reused and recycled, but at the same time, in order for this to also agree with non-toxic environment these closed loops should not contain hazardous chemicals. Hence, in our case this would mean that chemical A should not be used, based on its inherent toxicity, in order to achieve the non-toxic environment objective. This would however not fit into a circular economy (chemical A would now be a waste flow, as long as the production of the other chemicals from this process continues). Based on the result from our case study, there are no risks in our linear system, hence, it should be safe to include the use chemical A (in softener production) in circular loops. In fact, our result rather shows that while chemical A would be considered waste in scenario 2 (which as mentioned would not be in line with circular economy), this is not what contributes most to the overall impact. It is therefore evident, considering the result from both our assessments, that LCA and RA can be used to assess if changes intended to make the system be more in line with circular economy or non-toxic environment cause an improvement or not, in terms of increased or decreased negative externalities. They can also be used to evaluate the milestone targets for non-toxic environment.

In terms of circular economy LCA can, for example, include impact related to resource use, as well as assessing the impact of different sources of energy. In our LCA, we only assessed the replacement of two types of energy production with generated heat from incineration, but the decrease in impact from replacing fossil fuels (in the mixed electricity grid) to renewable energy can also be included. A change like this could for example, lower the climate change impact and indirect toxicity, which could lower the difference between softener A and softener B.

The implications of degradable materials will also be different in a circular economy and non-toxic environment. When it comes to hazardous chemicals, it is of course a good thing if they are degradable, to avoid bioaccumulation and biomagnification. However, if we want to use the chemicals in circular loops, degradation would significantly complicate things. For one, it could decrease the durability of the products it is integrated in, as well as recycling of the chemical would not be possible.

Unless there is a big change in consumption patterns, or if we manage to create perfectly closed circular flows, production of chemicals and so on will just continue to increase in the nearest future. As mentioned in background, only a small share of the chemicals produced and used today have been tested for inherent hazardous properties. One can assume that in the upcoming years, more and more chemicals will be tested and then have their use possibly restricted as a result. Companies will then need to perform assessment studies like RA to ensure that there are no risks to the people or environment caused by these chemicals. Substituting hazardous chemicals to safer alternatives might not always be easy. For example, in our case, chemical A is produced as a by-product and therefore production of it cannot cease without also stopping the manufacturing of the other chemicals made in that same process. Consequently, even if chemical A would be banned from use, production of it would still continue as long as all these other chemicals from this process are produced. As mentioned and analysed in this master thesis, another option could then be to incinerate chemical A and possibly utilise the generated heat in other processes, which could be a way to follow the circular economy framework in terms of that

all by-products should be used (i.e. no waste flows), and it could also replace fossil energy production. It is also important to consider that which softener is being used will depend on what type of fabric is being treated and what properties that is wanted in this fabric (for example different feel). Just exchanging one softener to another one might therefore not always be possible.

What is more important in the path to a more sustainable future: achieving a circular economy or a non-toxic environment? Can we argue whether or not resource use/circular flows are more valuable than risks to human health and the environment? The same discussion could be made if there would have been risks shown with chemical A. Then the choice would be between risk of direct toxicity and human health effects (chemical A) vs potential higher environmental impact, including indirect human health effects related to energy requirements (chemical B). How should one compare these? Are all risks to human health unacceptable? But even if so, impact on the environment (for example, through climate change) would also have an impact on human health (which can be accounted for in LCA by using weighting methods like DALY). However, one difference is that the environmental impact of a product and its involved processes can be lowered, by changing the type of energy sources, increasing resource efficiency, utilising surplus heat from other processes, etc. The risks to human health, or the environment, on the other hand would be more challenging to decrease, since lowering the exposure is not always possible.

The implications of a circular economy framework for chemical management/industrial companies, would be to work towards applying the following ideas: design durable products that can be used for a longer time, to make processes more resource efficient (reduce losses), use recycled material as inputs instead of virgin raw material, design their products in a way that enables and/or makes recycling easier, reduce waste flows and try to find uses of these materials (for example incineration and heat recovery), collaborate with other industrial companies to work towards industrial symbiosis (where outputs from one industry's process instead of being viewed as waste can be used as input for another industry's process). With chemical companies, while their products (the chemicals) might not be able to be designed as "recyclable", they can guide their downstream customers (that use "their" chemicals in manufacturing of products) to improve the recyclability of these products. Using renewable energy is also a possible way to comply with circular economy. In our case, if the textile wet treatment facility was using wind power instead of the modelled national grid in China, as has been used in this LCA, the climate change impact would be lower and consequently so would the difference between softener A and B.

In terms of non-toxic environment, companies can for example contribute by avoiding the use of hazardous chemicals when possible, and if chemicals with inherent hazardous properties are used, the companies should minimise the exposure to workers, consumers and environment. This can be done by using RA to analyse where the hotspots are, and hence where risk management is most urgently needed. This also applies to striving for both circular economy and toxic free environment; the materials to be recycled should not contain hazardous chemicals. Hence, analysis of these materials needs to be made to avoid hazardous residues. If using hazardous chemicals in manufacturing, with potential residues ending up in the final product, ways to reduce the level of residues should be investigated. It could potentially be possible to use

hazardous chemicals, when no safer alternative is available, as long as the exposure is limited throughout the chemical's and product's life cycles.

Based on our result, system thinking is important to avoid shifting of burden. Results like this (RA and LCA) could hopefully also be communicate to politicians and ecolabels, like bluesign, to show that it is important to have a systems perspective to avoid shifting of burden and that inherent hazards hence cannot be the only focus (which sometimes tends to be the case). While inherent hazardous properties of course are very important, the level of expected exposure should also be considered (however, it is not always possible to account for all possible exposures). As evident by the potential increase in environmental impact seen in the LCA, environmental impact should also be taken more into consideration. Possibly, when chemicals are restricted or banned, the possible alternatives should also be assessed, in order to see what consequences the restriction could bring. The results in this RA and LCA show that switching from softener A to softener B would result in a higher environmental impact. The case could also be that when one chemical is banned, the chemical that replaces it (which is not under restriction) could contribute to higher risks to human health. This could be a possibility, since there are many chemicals for which hazardous properties are not known. Evidently, this topic is a very complex one.

The result from these types of studies can be communicated to policy makers and other actors/stakeholders by using different types of media. For someone not familiar with assessment tools like LCA, aggregated results can be easier to grasp. One can also use graphs and figures to make the result more easily understood, and simplify the terms used. For example, instead of DNELs in the RA, terms such as safe levels or no effect levels can be used. One way of describing things in an easy way is by using videos. Then the concept of LCA, RA and other assessment tools can be described, as well as their results, through guiding the viewer with illustrations, etc. Explaining results in a video can be easier for the viewer to follow compared to reading about the result. Assessments like LCA and RA can be very extensive, and a lot of effort would be needed to make it completely understandable for the public not familiar with these concepts. Ecolabels are a way to communicate results to consumers; then the result is in most cases not even aggregated to a single number, the label itself is there to show the consumer if the textile for example do not contain any harmful substances. The more complicated the result that is communicated is, the higher is the risks that it can be misinterpreted.

In general, the communication and traceability are something that often can be improved throughout supply chains. However, as mentioned in the background, this is far from an easy task with complex and global supply value chains such as the case of the textile industry. In our case, information and data gaps were especially a problem for the downstream processes (such as the textile production, that includes use of softener in the textile wet treatment phases). For this thesis, we had contact with the softener producer, but they had limited information about the softener use in textile wet treatment, we hence recommend that contact with textile producers are to be made for future studies so that a more accurate modelling of the use of softeners in their processes is possible.

5.5 Other Limitations to the Master Thesis and Recommendations for Future Studies

As the reader of this master thesis report probably noticed, there were some things that we have had to exclude due to confidentiality, hence the transparency was somewhat limited. And since this thesis have been made in collaboration with a company, there is always a risk of being subjective. We of course have tried to avoid this and aimed to make the report as transparent as possible.

In the initial planning of the thesis, interviews with relevant key persons at Chalmers as well as the industry were included. However, other things in the thesis had to be prioritised. Future theses related to ours could look more into how companies in the textile value chain work with chemical risks, circular economy, etc. For example, interviews can be held with large actors in the textile sector and their suppliers. Another thesis could look more into the possibilities of calculating DALYs from RA in a way that they can be combined with DALYs from LCA. In the same way, endpoint for environmental burden can be looked into as well (potentially disappeared fraction of species (PDF)), as potentially, this can also be calculated from both LCA and RA to give another aspect to the comparison.

There are uncertainties when it comes to the softener use in textile wet treatment, and efforts have been made to clear these out. However, especially the water use/waste are uncertain and seems a bit unlikely. We recommend that in future studies contact should be made with the downstream actors from the softener producer. As of now, the usage is based on the softener producer's recommended dose, but there were also indications on that the dye house is usually using less softener than the recommended dosage. This communication would also aid in getting more accurate inventory data for the LCA on these processes. In general, more information about the softener molecules are wished for, as the current knowledge is very limited. Preferably, once more information about the softener can be established, it could eventually be possible to use DNELs and PNECs for the softeners and assess if it in themselves (and not just through chemical A/B residues) can cause a risk to human health or the environment. Analysis on to which extent chemical A/B and their softeners are washed out from the fabric (when the consumer washes the garment) should be made. Assessments on how much of the softener that can migrate from the clothes to the skin is also needed (for instance in regard to possible softener cleavage in the body). More studies on the chemical properties and identification of the softeners would also be needed to assess to what extent the softeners might cleave back into chemical A and B. A high level of cleavage would significantly increase the exposures to both humans and the environment. The water solubility of the softeners could be of importance when it comes to oral exposure of children (for example if cleavage to chemical A/B can be expected in the body). Potential metabolites formed in the body after exposure to chemical A, chemical B and their corresponding softeners, can also be of interest.

6. Conclusion

- The RA showed no RCR exceeding one for chemical A or B. The RCRs for consumers were very low. However, some RCRs were very close to one for some worker activities.
- The DNELs for systemic effects from long-term exposure indicate that chemical A has a higher long-term toxicity than chemical B.
- In the LCA, softener B showed slightly higher climate change impact than softener A, mainly due to higher temperature being needed to dissolve softener B.
- One way to combine LCA and RA frameworks is assessing risks over the life cycle (LCBRA) and adding more toxicity impact in LCA, by calculating (missing) characterisation factors with the help of RA.
- Results can be aggregated and expressed with the same unit, such as DALYs. This can also be done to make the result more tangible.
- DALYs from the LCA showed that scenario 1 (using 1 kg of softener A and 1 kg of softener B) was slightly more preferable than scenario 2 (using 2 kg of softener B and incinerating chemical A).
- Comparing DALY from LCA and RA can be done, but then have to be on the same basis. The level of uncertainty has to be taken into account.
- Assessment tools like RA and LCA can be used to analyse how companies' products and processes fit into the circular economy and toxic free environment concepts.
- Both types of assessments are needed to avoid problem shifting, as they cover different aspects (for example, safety is only assessed in RA).

6.1Recommendations for Future Studies

- Further contact with downstream actors are recommended in order to get more accurate information regarding:
    - PROC and PPE assumptions for manufacturing of the two chemicals, softener production and dye house, so that the assumptions correctly describe their actual processes.
    - Information about the doses of softener used.
    - Information about water use, to get a more accurate model of the textile wet treatment.
    - Information about emissions and wastewater, so that more site-specific environmental exposure (RA) and more accurate impacts (LCA) can be done (using more site-specific emission data instead of EFs from ERCs).
    - Site-specific data for LCA to get more accurate data related to electricity and heating in dye house and incineration of chemical A in China.
    - Information on how many people that are working in factories, amount of chemical/softener produced or used per day etc. and how much clothes are treated with these softeners (compared to "total market") are needed to be able to estimate possible exposure (for calculating DALYs from RA in possible future study).

- More case-specific exposure of workers, by either adjusting ECETOC or use a different tool, to take chemical properties, concentration ranges and other aspects more accurately into account.
- Calculation of missing DNELs.
- Calculate exposure to retailers. For this, exposure through dust particles (chemical A and B on textile fibres) can be of interest as an additional exposure route.
- Regarding no effect levels, to look further at existing studies and possibly more animal studies are needed:
    - For chemical A to get more certain no effect level.
    - For chemical B, while toxicity to reproduction was ruled out in an animal study, the dose at which other types of effects were seen could be basis for other toxicity studies.
- Possible future theses:
    - How DALYs can be calculated based on RA and how to construct this in a way that it is comparable with DALYs from LCA.
    - Comparing LCA and RA using an endpoint for environmental burden (PDF).
    - Performing interviews with actors such as clothing companies, dye houses, universities and politicians, to see how the view on toxicity of chemicals in products used on textiles differs between different actors and different parts of the textile value chain, and how information about toxicity is currently communicated between them.
- More information on softener A and B is needed, for which studies on their properties such as composition, biodegradability, toxicity, water solubility, cleavage etc. are desirable.
- Attributional LCA that also considers the textile life cycle, and all other chemicals used in relation to this, to see the impact of softener relative to this total impact.

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8. Appendix

8.1 DNELs

DNELs used in our RA and what endpoint these are based on can be seen in the following tables.

8.1.1 Chemical A

Workers:

Hazard via...			**DNEL**	**Most sensitive endpoint**
Inhalation route	Systemic effects	*Long term exposure*	**0.7 mg/m^3**	Developmental toxicity/teratogenicity
		Acute/short term exposure	No hazard identified	
	Local effects	*Long term exposure*	Medium hazard (no threshold derived)	Skin irritation/corrosion
		Acute/short term exposure	Medium hazard (no threshold derived)	Skin irritation/corrosion
Dermal route	Systemic effects	*Long term exposure*	**2 mg/kg bw/day**	Developmental toxicity/teratogenicity
		Acute/short term exposure	No hazard identified	
	Local effects	*Long term exposure*	**30 µg/cm^2** (AkzoNobel, 2013)	(dermal subacute study)
		Acute/short term exposure	Medium hazard (no threshold derived)	Skin irritation/corrosion

Eyes	Local effects	High hazard (no threshold derived)	

General population:

Hazard via...			**DNEL**	**Most sensitive endpoint**
Inhalation route	Systemic effects	Long term exposure	**0.2 mg/m^3**	Developmental toxicity/teratogenicity
		Acute/short term exposure	No hazard identified	
	Local effects	Long term exposure		
		Acute/short term exposure		
Dermal route	Systemic effects	Long term exposure	**1 mg/kg bw/day**	Developmental toxicity/teratogenicity
		Acute/short term exposure		
	Local effects	Long term exposure	**20 µg/cm^2** (AkzoNobel, 2013)	(From dermal sub-acute study)
		Acute/short term exposure		
Oral route	Systemic effects	Long term exposure	**0.1 mg/kg bw/day**	Developmental toxicity/teratogenicity
		Acute/short term exposure		
	Local effects	Long term	**1 mg/kg bw/day**	(from oral sub-acute

			(AkzoNobel, 2013)	study)
		Acute/short term		
Eyes	Local effects			

8.1.2 Chemical B

Workers:

Hazard via...			**DNEL**	**Most sensitive endpoint**
Inhalation route	Systemic effects	*Long term exposure*	**20 mg/m^3**	Repeated dose toxicity
		Acute/short term exposure	**90 mg/m^3**	Repeated dose toxicity
	Local effects	*Long term exposure*	**0.9 mg/m^3**	Acute toxicity
		Acute/short term exposure	**3 mg/m^3**	Acute toxicity
Dermal route	Systemic effects	*Long term exposure*	**11 mg/kg bw/day**	Repeated dose toxicity
		Acute/short term exposure	Exposure based waiving	
	Local effects	*Long term exposure*	**1 mg/cm^2**	Repeated dose toxicity
		Acute/short term exposure	Exposure based waiving	
Eyes	Local effects		No hazard identified	

General population:

Hazard via...			**DNEL**	**Most sensitive endpoint**
Inhalation route	Systemic effects	*Long term exposure*	**5 mg/m^3**	Repeated dose toxicity
		Acute/short term exposure	**30 mg/m^3**	Repeated dose toxicity
	Local effects	*Long term exposure*	Exposure based waiving	
		Acute/short term exposure	Exposure based waiving	
Dermal route	Systemic effects	*Long term exposure*	**5 mg/kg bw/day**	Repeated dose toxicity
		Acute/short term exposure	**5 mg/kg bw/day**	Repeated dose toxicity
	Local effects	*Long term exposure*	Exposure based waiving	
		Acute/short term exposure	Exposure based waiving	
Oral route	Systemic effects	*Long term exposure*	Exposure based waiving	
		Acute/short term exposure	Exposure based waiving	
	Local effects	*Long term exposure*		
		Acute/short term exposure		
Eyes	Local effects		No hazard identified	

8.2 Exposure to workers

The table below presents the PROCs used for the involved processes. Grey box indicates that the PROC is used for this process. (For the full name and explanation of each PROC, please refer to ECHA (2015).)

PROC	Name	Manufacturing of chemical A/B:	Production of softener:	Use of softener:
1	Chemical production in closed process without the likelihood of exposure			
2	Chemical production in closed continuous process with occasional controlled exposure			
3	Manufacture in the chemical industry in closed batch processes with occasional controlled exposures			
4	Chemical production where opportunity for exposure arises			
5	Mixing or blending in batch processes			
6	Calendering operations			
8a	Transfer of substance or mixture at non-dedicated facilities			
8b	Transfer of substance or mixture at dedicated facilities			
9	Transfer of substance or mixture into small containers			
10	Roller application or brushing			
13	Treatment of articles by dipping and pouring			
15	Use as laboratory reagent			

The resulting calculated exposure is presented in the following sections, divided into each process and the different PROCs for the activities therein.

8.2.1 Manufacturing of Chemical A and B

Chemical A:

	Long-term Inhalative Exposure Estimate (ppm for volatiles) / (mg/m^3 for solids)	Long-term Inhalative Exposure Estimate (mg/m^3)	Long-term Dermal Exposure Estimate (mg/kg/day)	Short-term Inhalative Exposure Estimate (mg/m^3)	Local Dermal Exposure Estimate ($\mu g/cm^2$)
PROC 1	0,010	0,043	0,034	0,174	10,000
PROC 2	0,100	0,434	0,137	1,740	20,000
PROC 8a	0,100	0,434	0,274	1,740	20,000
PROC 8b	0,075	0,325	0,137	1,300	10,000
PROC 15	0,150	0,651	0,069	2,600	20,000

Chemical B:

	Long-term Inhalative Exposure Estimate (ppm for volatiles) / (mg/m^3 for solids)	Long-term Inhalative Exposure Estimate (mg/m^3)	Long-term Dermal Exposure Estimate (mg/kg/day)	Short-term Inhalative Exposure Estimate (mg/m^3)	Local Dermal Exposure Estimate ($\mu g/cm^2$)
PROC 1	0,010	0,043	0,034	0,172	10,000
PROC 2	0,100	0,430	0,137	1,720	20,000
PROC 8a	0,100	0,430	0,274	1,720	20,000
PROC 8b	0,075	0,322	0,137	1,290	10,000
PROC 15	0,150	0,645	0,069	2,580	20,000

8.2.2. Production of Softener

Chemical A:

	Long-term Inhalative Exposure Estimate (ppm for volatiles) / (mg/m^3 for solids)	Long-term Inhalative Exposure Estimate (mg/m^3)	Long-term Dermal Exposure Estimate (mg/kg/day)	Short-term Inhalative Exposure Estimate (mg/m^3)	Local Dermal Exposure Estimate ($\mu g/cm^2$)
PROC 1	0,010	0,043	0,034	0,174	10,000
PROC 2	0,100	0,434	0,137	1,740	20,000
PROC 3	0,090	0,391	0,069	1,560	20,000
PROC 4	0,150	0,651	0,137	2,600	20,000
PROC 5	0,150	0,651	0,137	2,600	20,000
PROC 8a	0,030	0,130	0,274	0,521	20,000
PROC 8b	0,075	0,325	0,137	1,300	10,000
PROC 9	0,150	0,651	0,137	2,600	20,000

Chemical B:

	Long-term Inhalative Exposure Estimate (ppm for volatiles) / (mg/m^3 for solids)	Long-term Inhalative Exposure Estimate (mg/m^3)	Long-term Dermal Exposure Estimate (mg/kg/day)	Short-term Inhalative Exposure Estimate (mg/m^3)	Local Dermal Exposure Estimate ($\mu g/cm^2$)
PROC 1	0,010	0,043	0,034	0,172	10,000
PROC 2	0,100	0,430	0,137	1,720	20,000
PROC 3	0,090	0,387	0,069	1,550	20,000
PROC 4	0,150	0,645	0,137	2,580	20,000
PROC 5	0,150	0,645	0,137	2,580	20,000
PROC 8a	0,030	0,129	0,274	0,516	20,000
PROC 8b	0,075	0,322	0,137	1,290	10,000
PROC 9	0,150	0,645	0,137	2,580	20,000

8.2.3 Use of Softener

Chemical A:

	Long-term Inhalative Exposure Estimate (ppm for volatiles) / (mg/m^3 for solids)	Long-term Inhalative Exposure Estimate (mg/m^3)	Long-term Dermal Exposure Estimate (mg/kg/day)	Short-term Inhalative Exposure Estimate (mg/m^3)	Local Dermal Exposure Estimate ($\mu g/cm^2$)
PROC 6	0,150	0,651	0,274	2,600	20,000
PROC 8a	0,100	0,434	0,274	1,740	20,000
PROC 10	0,100	0,434	0,274	1,740	20,000
PROC 13	0,100	0,434	0,137	1,740	20,000

Chemical B:

	Long-term Inhalative Exposure Estimate (ppm for volatiles) / (mg/m^3 for solids)	Long-term Inhalative Exposure Estimate (mg/m^3)	Long-term Dermal Exposure Estimate (mg/kg/day)	Short-term Inhalative Exposure Estimate (mg/m^3)	Local Dermal Exposure Estimate ($\mu g/cm^2$)
PROC 6	0,150	0,645	0,274	2,580	20,000
PROC 8a	0,100	0,430	0,274	1,720	20,000
PROC 10	0,100	0,430	0,274	1,720	20,000
PROC 13	0,100	0,430	0,137	1,720	20,000

8.3 Risk Characterisation Ratios to Workers

The calculated RCRs will be presented in the following sections.
Colour coding used in the tables:

RCR < 0,5
0,5 < RCR < 0,75
0,75 < RCR < 1
RCR > 1

Table of risk characterisation ratios, for the different life cycle processes. The numbers in the tables are the highest risk characterisation ratio for each process. For the risk characterisation ratios for each PROC within the processes, see further below.

			Manufacturing of chemical A and B		**Production of softener**		**Use of softener**	
Type of exposure:			*Chemical A*	*Chemical B*	*Chemical A*	*Chemical B*	*Chemical A*	*Chemical B*
Inhalation	Systemic	Long term	0,925	0,042	0,925	0,042	0,925	0,042
		Short term		0,028		0,028		0,028
	Local	Long term		0,741		0,741		0,741
		Short term		0,992		0,992		0,992
Dermal	Systemic	Long term	0,137	0,024	0,137	0,024	0,137	0,024
		Short term						
	Local	Long term	0,80	0,018	0,80	0,018	0,80	0,018
		Short term						
Eyes	Local							

8.3.1 Manufacturing of Chemical A and B:

Chemical A:

Exposure via...			PROC 1	PROC 2	PROC 8a	PROC 8b	PROC 15
Inhalation	Systemic	Long term	0,062	0,616	0,616	0,462	0,925
		Short term					
	Local	Long term					
		Short term					
Dermal	Systemic	Long term	0,017	0,069	0,137	0,069	0,034
		Short term					
	Local	Long term	0,400	0,800	0,800	0,400	0,800
		Short term					
Eyes	Local						

Chemical B:

Exposure via...			PROC 1	PROC 2	PROC 8a	PROC 8b	PROC 15
Inhalation	Systemic	Long term	0,003	0,028	0,028	0,021	0,042
		Short term	0,002	0,019	0,019	0,014	0,028
	Local	Long term	0,049	0,494	0,494	0,370	0,741
		Short term	0,066	0,662	0,662	0,496	0,992
Dermal	Systemic	Long term	0,003	0,012	0,024	0,012	0,006
		Short term					
	Local	Long term	0,009	0,018	0,018	0,009	0,018
		Short term					
Eyes	Local						

8.3.2 Production of Softener:

Chemical A:

Exposure via...			PROC 1	PROC 2	PROC 3	PROC 4	PROC 5	PROC 8a	PROC 8b	PROC 9
Inhalation	Systemic	Long term	0,062	0,616	0,555	0,925	0,925	0,185	0,462	0,925
		Short term								
	Local	Long term								
		Short term								
Dermal	Systemic	Long term	0,017	0,069	0,034	0,069	0,069	0,137	0,069	0,069
		Short term								
	Local	Long term	0,400	0,800	0,800	0,800	0,800	0,800	0,400	0,800
		Short term								
Eyes	Local									

Chemical B:

Exposure via...			PROC 1	PROC 2	PROC 3	PROC 4	PROC 5	PROC 8a	PROC 8b	PROC 9
Inhalation	Systemic	Long term	0,003	0,028	0,025	0,042	0,042	0,008	0,021	0,042
		Short term	0,002	0,019	0,017	0,028	0,028	0,006	0,014	0,028
	Local	Long term	0,049	0,494	0,445	0,741	0,741	0,148	0,370	0,741
		Short term	0,066	0,662	0,596	0,992	0,992	0,198	0,496	0,992
Dermal	Systemic	Long term	0,003	0,012	0,006	0,012	0,012	0,024	0,012	0,012
		Short term								
	Local	Long term	0,009	0,018	0,018	0,018	0,018	0,018	0,009	0,018
		Short term								
Eyes	Local									

8.3.3 Use of Softener

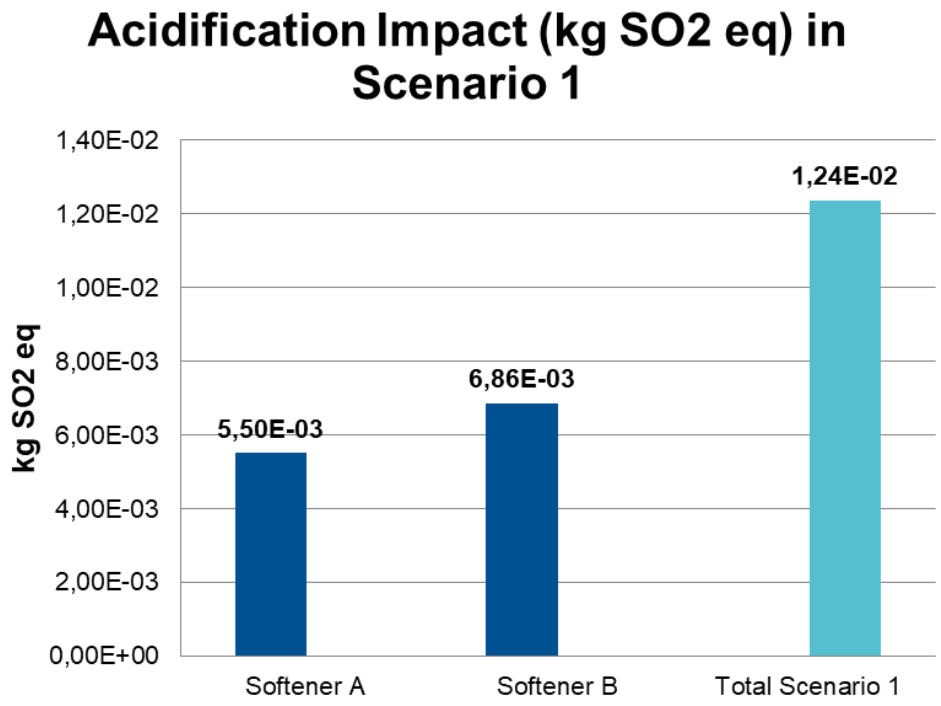
Chemical A:

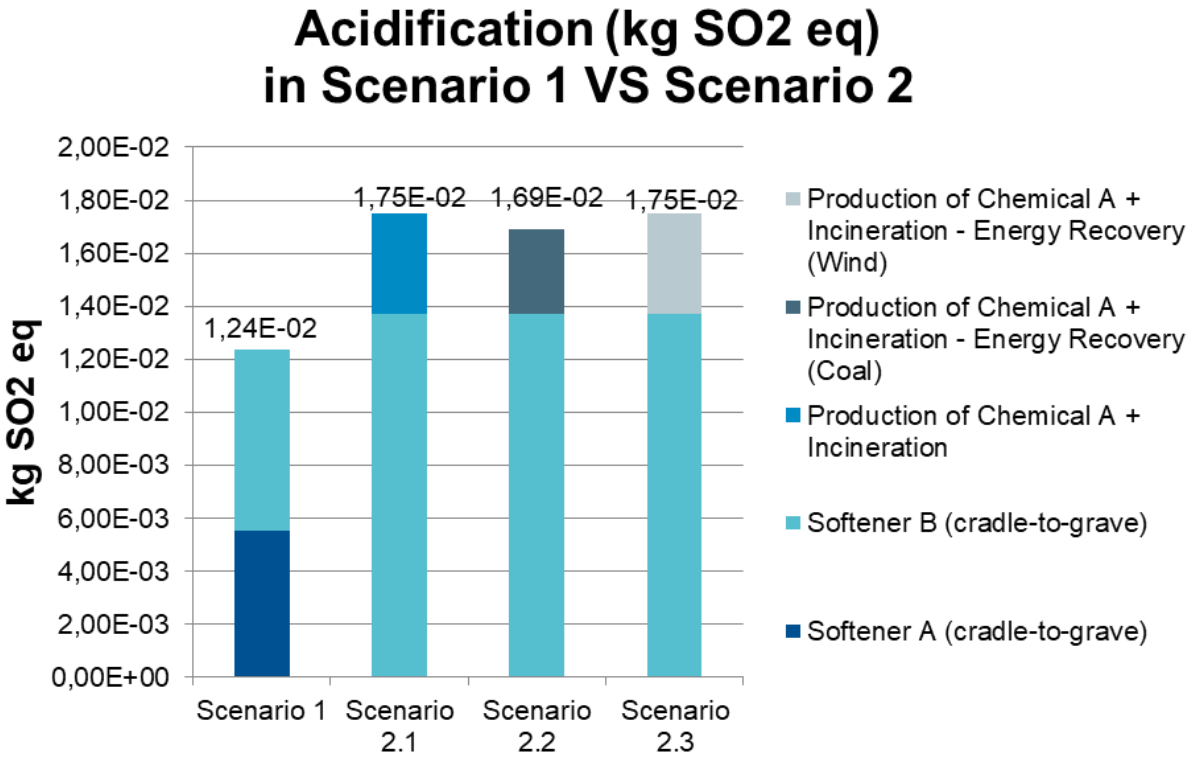
Exposure via...			PROC 6	PROC 8a	PROC 10	PROC 13
Inhalation	Systemic	Long term	0,925	0,616	0,616	0,616
		Short term				
	Local	Long term				
		Short term				
Dermal	Systemic	Long term	0,137	0,137	0,137	0,069
		Short term				
	Local	Long term	0,800	0,800	0,800	0,800
		Short term				
Eyes	Local					

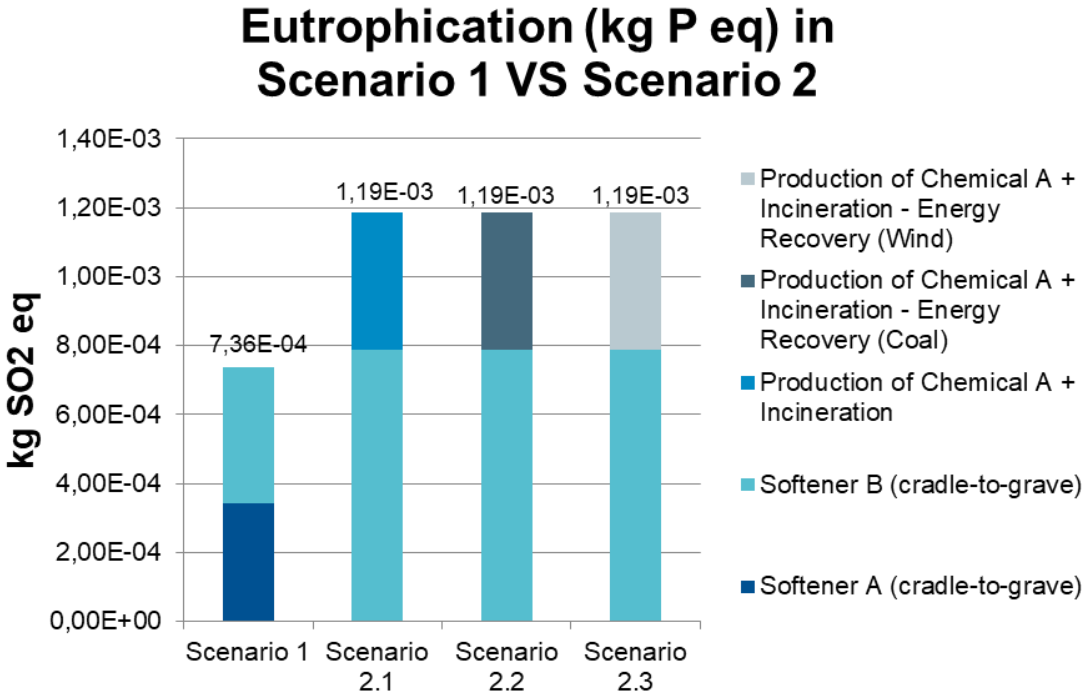
Chemical B:

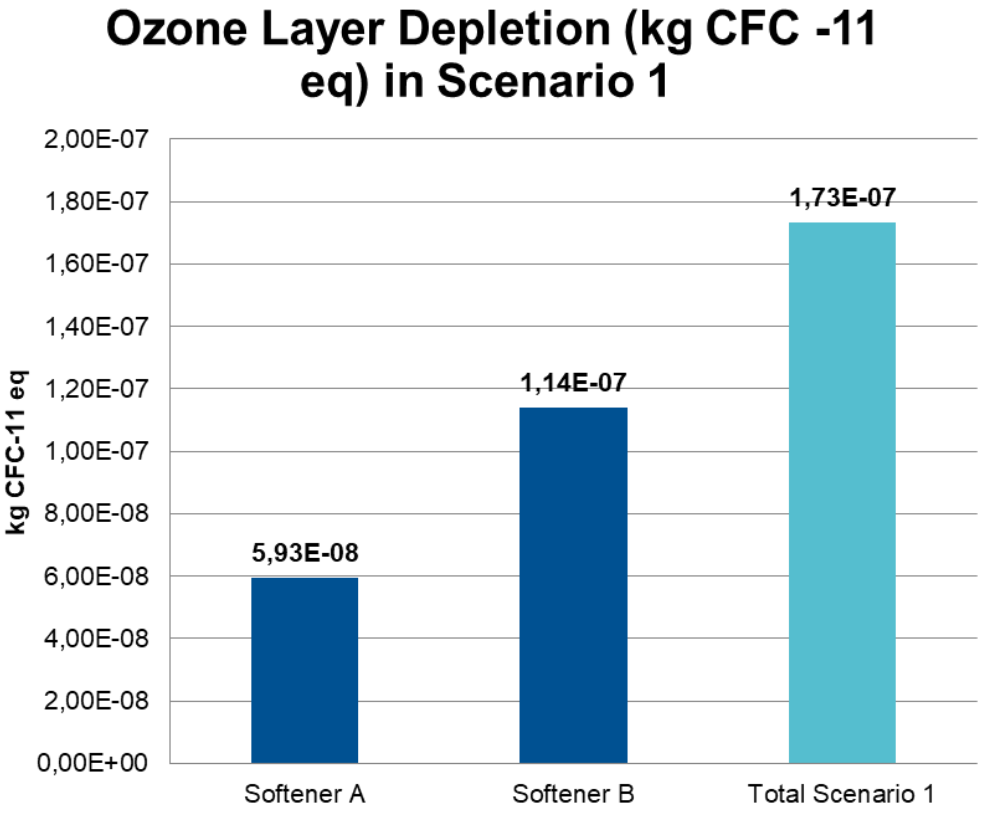
Exposure via...			PROC 6	PROC 8a	PROC 10	PROC 13
Inhalation	Systemic	Long term	0,042	0,028	0,028	0,028
		Short term	0,028	0,019	0,019	0,019
	Local	Long term	0,741	0,494	0,494	0,494
		Short term	0,992	0,662	0,662	0,662
Dermal	Systemic	Long term	0,024	0,024	0,024	0,012
		Short term				
	Local	Long term	0,018	0,018	0,018	0,018
		Short term				
Eyes	Local					

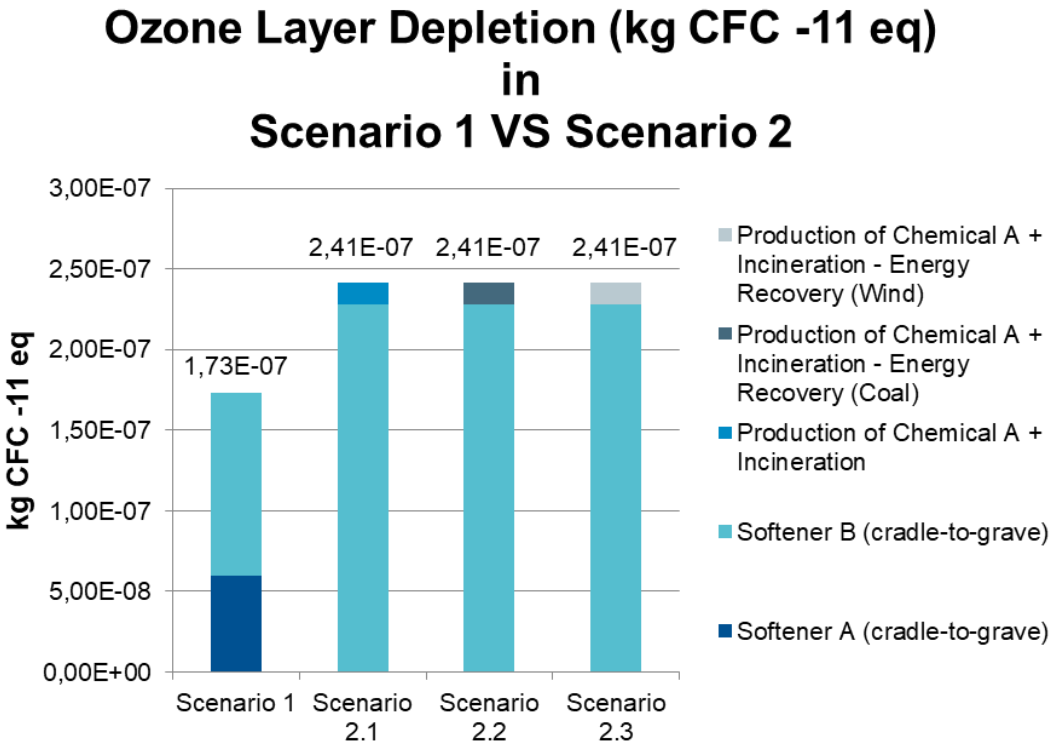
8.4 Life Cycle Impact

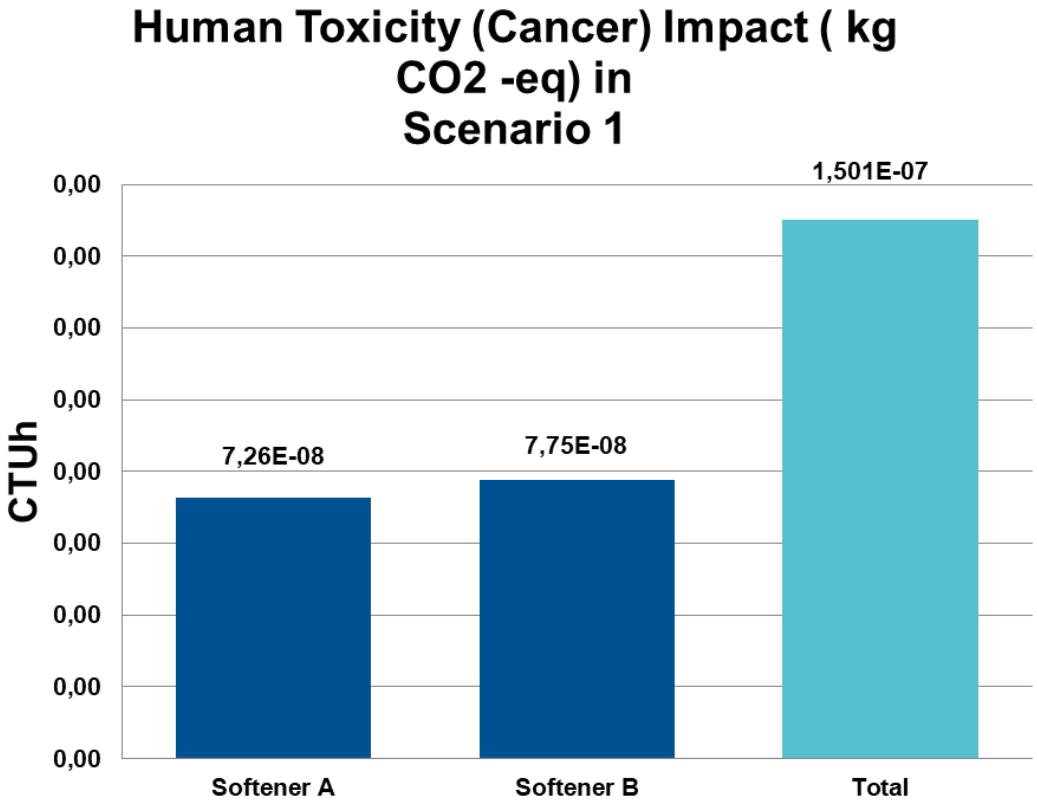


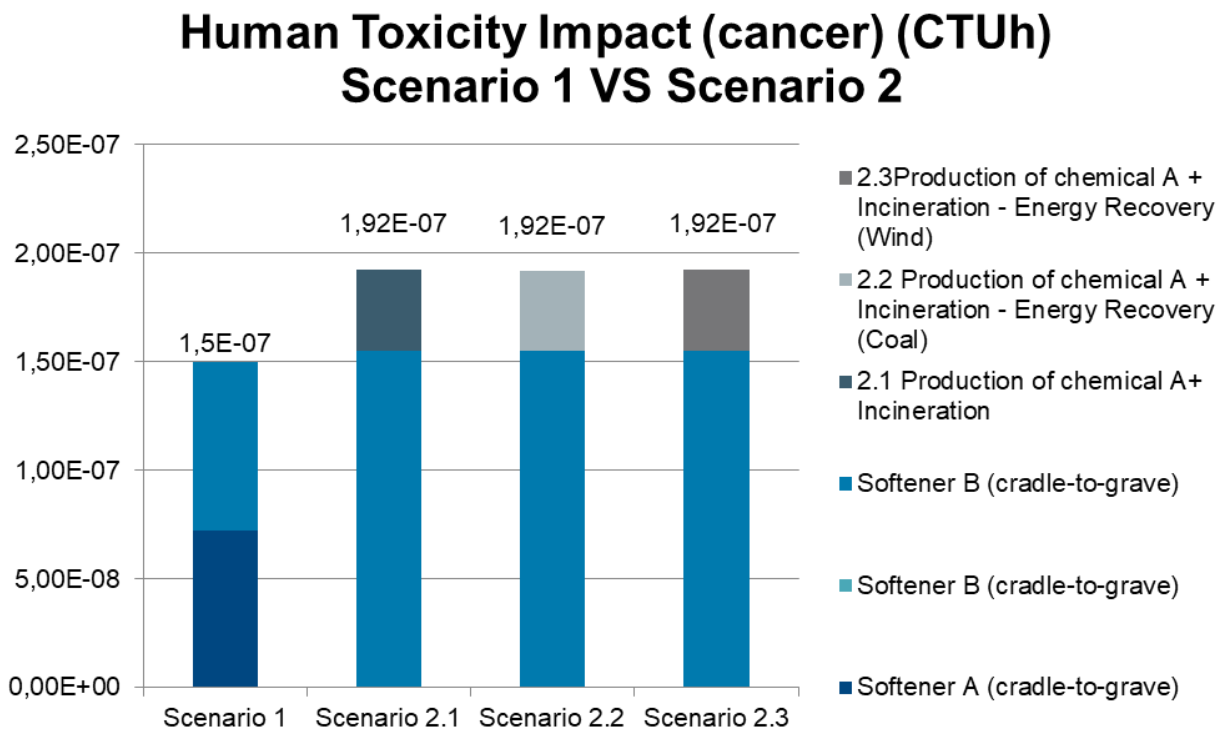



Eutrophication (kg P eq) in Scenario 1 VS Scenario 2
kg SO2 eq
1,40E-03
1,20E-03
1,00E-03
8,00E-04
6,00E-04
4,00E-04
2,00E-04
0,00E+00
7,36E-04
1,19E-03
1,19E-03
1,19E-03
Scenario 1
Scenario 2.1
Scenario 2.2
Scenario 2.3
Production of Chemical A + Incineration - Energy Recovery (Wind)
Production of Chemical A + Incineration - Energy Recovery (Coal)
Production of Chemical A + Incineration
Softener B (cradle-to-grave)
Softener A (cradle-to-grave)


Ozone Layer Depletion (kg CFC -11 eq) in Scenario 1
kg CFC-11 eq
2,00E-07
1,80E-07
1,60E-07
1,40E-07
1,20E-07
1,00E-07
8,00E-08
6,00E-08
4,00E-08
2,00E-08
0,00E+00
5,93E-08
1,14E-07
1,73E-07
Softener A
Softener B
Total Scenario 1


Ozone Layer Depletion (kg CFC -11 eq) in Scenario 1 VS Scenario 2
kg CFC -11 eq
3,00E-07
2,50E-07
2,00E-07
1,50E-07
1,00E-07
5,00E-08
0,00E+00
1,73E-07
2,41E-07
2,41E-07
2,41E-07
Scenario 1
Scenario 2.1
Scenario 2.2
Scenario 2.3
Production of Chemical A + Incineration - Energy Recovery (Wind)
Production of Chemical A + Incineration - Energy Recovery (Coal)
Production of Chemical A + Incineration
Softener B (cradle-to-grave)
Softener A (cradle-to-grave)


Human Toxicity (Cancer) Impact (kg CO2 -eq) in Scenario 1
CTUh
0,00
0,00
0,00
0,00
0,00
0,00
0,00
0,00
0,00
7,26E-08
7,75E-08
1,501E-07
Softener A
Softener B
Total


Human Toxicity Impact (cancer) (CTUh)
Scenario 1 VS Scenario 2
2,50E-07
2,00E-07
1,50E-07
1,00E-07
5,00E-08
0,00E+00
1,5E-07
1,92E-07
1,92E-07
1,92E-07
Scenario 1
Scenario 2.1
Scenario 2.2
Scenario 2.3
2.3Production of chemical A + Incineration - Energy Recovery (Wind)
2.2 Production of chemical A + Incineration - Energy Recovery (Coal)
2.1 Production of chemical A+ Incineration
Softener B (cradle-to-grave)
Softener B (cradle-to-grave)
Softener A (cradle-to-grave)