# LIFE CYCLE ASSESSMENT FOR WASTEWATER DISINFECTION USING SODIUM HYPOCHLORITE, PERACETIC ACID OR PERFORMIC ACID

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## Abstract

As the need for safe water is increasing, engineers are working on finding more efficient and environment-friendly technologies for disinfection of wastewater in order to provide safe water for discharge into the environment. Chlorination, using sodium hypochlorite (NaOCl), is one of the most commonly used disinfection methods. In recent years, extensive research has been done on performic (PFA) and peracetic acid (PAA), as they have a high oxidation potential and therefore can reduce bacterial and other types of contamination in wastewater.

Life Cycle Assessment (LCA) is a holistic method used in order to investigate the environmental footprint of a product or a service over its entire life cycle, i.e. from "cradle-to-grave".

The objective of the thesis is to use LCA to demonstrate the advantages in using either NaOCl, PAA or PFA for wastewater disinfection, from an environmental and health perspective.

USEtox and Impact 2002+ models were used in order to evaluate their impacts on freshwater toxicity, human toxicity, climate change, mineral resources and non-renewable energy depletion. Data for the study were provided by a treatment plant in Italy near Venice that has performed full-scale disinfection trials using NaOCl, PAA and PFA, and by the North West Langley treatment plant near Vancouver, which traditionally used NaOCl for chlorination and sodium bisulfite for dechlorination, but transitioned to PAA disinfection in 2014.

The functional unit for the Venice treatment plant is the removal of 3 log of *E. coli* from the effluent at a flow of 27 MLD during two months. For the NW Langley treatment plant, the functional unit was the disinfection of the effluent to the limit of 200 MPN/100 ml fecal coliforms at the edge of the dilution zone, from April to October and at a flow of 11.5 MLD. The LCA includes chemical production, infrastructure directly related to disinfection at the treatment plant, ancillary equipment for disinfection, transportation of equipment and the disinfectants, electricity for disinfection process itself as well as the residuals from disinfection.

Results from the Venice treatment plant indicate that PFA could be the best option for wastewater disinfection due to the low dose needed to achieve regulatory limits, which reduces the potential impact of chemical production as well as transport. While PFA is more toxic than PAA, the residual concentration is lower leading to similar potential impacts on toxicity. Results from the NW Langley WWTP indicate that dechlorination significantly reduces potential

impacts of chlorine on freshwater toxicity, however impacts on human toxicity, climate change and resource consumption (mineral and non-renewable energy) are increased due to the added production and transport of sodium bisulfite.

The best choice of disinfectant at NW Langley therefore depends on the environmental priorities of the decision makers and government regulations. For each disinfectant, production is the highest contributor to total potential impacts on climate change, human toxicity and resource depletion. The highest contributor to freshwater toxicity impacts is the chemical residual from disinfection.

The choice of chemical disinfectant also depends on regulations, cost and technologies available. The DesinFix unit is only being used in Europe; at this time the US EPA and the Canadian government have not yet approved the use of PFA for wastewater disinfection. Nonetheless, with upcoming reviews in regulations, PFA could soon be available in more countries. Furthermore, a cost analysis would give more information on the economic benefits of using one disinfectant over another.

**Résumé**

L'augmentation de la demande en eau potable partout au monde amène les ingénieurs à chercher des solutions techniques plus efficaces et propres pour l'environnement afin de s'assurer que les eaux usées peuvent être rejetées en toute sécurité et sans affecter la santé publique. L'utilisation du chlore sous la forme d'hypochlorite de sodium est une des méthodes les plus courantes au niveau mondial. Depuis quelques années, on observe une augmentation de la recherche scientifique sur les acides performique et peracétique pour la désinfection. Ces composés représentent des alternatives ayant un potentiel d'oxydation élevé et pouvant donc lutter efficacement contre la présence de bactéries et d'autres contaminants dans les eaux usées.

L'analyse du cycle de vie (ACV) est une méthode holistique utilisée afin de déterminer l'impact sur l'environnement d'un produit ou d'un service en considérant son cycle de vie en entier.

L'objectif de ce mémoire est d'utiliser l'ACV afin de déterminer les avantages à utiliser l'hypochlorite de sodium, l'acide performique ou l'acide peracétique pour la désinfection des eaux usées, du point de vue des impacts sur l'environnement et la santé.

Les modèles USEtox et Impact 2002+ ont été utilisés afin d'évaluer les impacts des désinfectants sur la toxicité aquatique, la toxicité humaine, les changements climatiques, l'utilisation de ressources minérales et d'énergies non-renouvelables. Les données de l'étude proviennent de deux usines de traitement des eaux usées : la première située en Italie, près de la ville de Venise qui a utilisé les trois produits pour la désinfection à grande échelle, et la deuxième la North West Langley située près de la ville de Vancouver au Canada. Cette dernière a utilisé l'hypochlorite de sodium avec déchloration pendant plusieurs années, mais utilise l'acide peracétique depuis l'été 2014.

L'unité fonctionnelle utilisée pour l'usine de Venise est l'élimination de 3 log d'*E. coli* de l'effluent de l'usine à un débit de 27 MLD pendant deux mois. Pour l'usine de Vancouver, l'unité fonctionnelle est la désinfection des eaux usées à la norme canadienne de 200 MPN/100 ml de coliformes fécaux à la limite de la zone de mélange, d'avril à octobre et à un débit de 11.5 MLD. L'ACV considère les étapes de production des désinfectants, des infrastructures utilisées pour la désinfection et des équipements nécessaires, ainsi que le transport d'équipements et de produits chimiques, la désinfection et les résidus restants dans l'effluent.

Les résultats obtenus pour l'usine de Venise indiquent que l'acide performique serait la meilleure option pour la désinfection des eaux usées et ce grâce à la plus petite dose de produit chimique nécessaire afin de réduire la contamination à la limite permise, ce qui diminue les impacts du transport et de la production chimique. L'acide performique possède une plus grande toxicité aquatique que l'acide peracétique, toutefois le résiduel est moins important : l'impact final des deux produits est donc semblable. Les résultats obtenus à l'usine de Vancouver indiquent que la déchloration avec bisulfite de sodium diminue les impacts sur la toxicité aquatique de façon significative. Toutefois, les impacts potentiels sur la toxicité humaine, les changements climatiques et l'utilisation des ressources sont plus importants, et ce dû à la production chimique et au transport supplémentaire nécessaires. Le meilleur choix, considérant les impacts potentiels, de produit de désinfection à l'usine de Vancouver dépend donc des priorités environnementales des décideurs et des normes environnementales existantes. Pour tous les désinfectants, la production chimique est l'élément qui contribue le plus aux impacts potentiels sur les changements climatiques, la toxicité humaine et l'utilisation des ressources minérales et non-renouvelables, alors que l'impact sur la toxicité aquatique est dû en majorité au résiduel de désinfection.

Le choix du désinfectant à utiliser dépend également des règlements et normes, des technologies disponibles et du coût associé. Par exemple, l'utilisation de l'acide performique n'est pas encore acceptée par les gouvernements du Canada et des États-Unis. Toutefois, avec le temps, son utilisation devrait être de plus en plus acceptée. Afin de compléter cette étude une analyse de coût permettrait de fournir plus d'informations sur les avantages et inconvénients à utiliser un désinfectant plutôt qu'un autre.

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# 1. Introduction

## 1.1 Background

As the need for safe water is increasing with the rising world population, engineers are working on finding more efficient and environment-friendly technologies for disinfection of wastewater in order to provide safe water for discharge into the environment. Many different technologies have been developed, based on physical, biological and/or chemical treatment. Chlorination, using sodium hypochlorite (NaOCl) or other forms of chlorine, is one of the most commonly used disinfection methods. In recent years, extensive research has been done on performic and peracetic acid, as they have a high oxidation potential and therefore can reduce bacterial and other types of contamination in wastewater.

Peracetic acid (PAA, $CH_3CO_3H$) is used extensively in the food, beverage and medical industries and is produced by reacting acetic acid with hydrogen peroxide in the presence of a catalyst. Due to its high reactivity, PAA breaks back down into acetic acid (vinegar) and hydrogen peroxide very quickly and therefore is not a danger to the aquatic environment downstream from treatment plants. Finally, it is simple for wastewater treatment plants to transition from chlorine use (which may produce harmful disinfection by-products and adversely affect aquatic life) as chlorine contact chambers may be retrofitted for use with PAA (Santoro et al., 2017). The disadvantage of PAA use is an increased organic content in the effluent, which could cause local algae growth downstream from injection. Furthermore, a limited production capacity worldwide of PAA has increased its cost (Voukkali & Zorpas, 2014).

Performic acid (PFA, $CH_2O_3$) is produced on-site, by combining hydrogen peroxide and formic acid. Also used in fields other than wastewater treatment for many years, its use is more recent than that of peracetic acid, having been made commercially available in quantities large enough for wastewater treatment only recently. Less is known, in terms of toxicity and by-products formed, about performic acid compared to peracetic acid. Safety concerns are more important for performic acid, as it becomes very unstable at high temperatures and concentrations (Luukkonen et al. 2015).

Sodium hypochlorite (NaOCl) is one of the most widely used methods of wastewater disinfection and presents many advantages to alternatives: it is cost-efficient, reliable and efficient. Furthermore, a residual remains in the water, which insures continued disinfection after application. However, chlorine is toxic to aquatic life and forms harmful by-products even at concentrations as low as 0.04 mg/L (United States Environmental Protection Agency (US EPA), 1999, 1992). To protect aquatic life, a dechlorination step is often added to the disinfection system (US EPA, 2000).

Life Cycle Assessment (LCA) is a holistic method, which has been in development since the 1970s. It is used in order to investigate the environmental footprint of a product or a service over its entire life cycle, i.e. from "cradle-to-grave". It serves two major purposes: First, to identify possible environmental "hotspots" in the life cycle, and second, to compare different products or services in order to determine which alternative has a smaller environmental potential impact. Life cycle assessments must contain an impact assessment, which helps determine where the potential impacts of the product or service analysed are concentrated. Life cycle assessment can also be used to evaluate potential impacts on human health, as impacts on the environment generally also affect humans.

Using LCA has the advantage of avoiding the displacement of impacts (Joliett et al. 2015). Comparing products or processes based only on their use or the end of life, for example, omits the entire fabrication process, which can be an important contributor to potential environmental impacts. By using LCA, all potential impacts throughout the life cycle are included.

LCA is one of the best tools available for demonstrating the advantages in using either chlorine, peracetic acid or performic acid for wastewater disinfection, from an environmental perspective. Life cycle assessment is also used for cost analysis in order to improve the design of products and reduce design changes, cost and time to market (Asiedu & Gu, 1998). This study, however, will focus on evaluating environmental and human impacts only.

## 1.2 Objectives of the study

The major objective of the study is to do a life cycle assessment of three different methods of wastewater disinfection in order to determine which alternative has the smallest potential environmental impact from a cradle-to-grave perspective. The treatment methods chosen for this study are all tertiary disinfection alternatives that follow secondary treatment of wastewater: (1) sodium hypochlorite, (2) peracetic acid, and (3) performic acid. A secondary objective is to create a general framework for future use and application to specific treatment plants in order to determine the potential impacts of each technology at a specific location.

# 2. Literature review

## 2.1 Wastewater disinfection

The main objectives of wastewater disinfection are to reduce the risk of recreational users from being exposed to pathogens in surface waters, and to limit the risk of the source water of a drinking water treatment plant being contaminated by the effluent of an upstream wastewater treatment plant (Droste & Gehr, 2018). The most common microorganisms found in wastewater include enteric bacteria, viruses and protozoan cysts.

Traditionally, chlorine disinfection was used in most treatment plants, however, in recent years many alternatives to chlorine have been developed. The main downside to using chlorine for wastewater disinfection is the toxicity of chlorine residuals being released into receiving environments through the treatment plant effluent. This has led many countries to regulate the chlorine concentration of treatment plant effluents, and in some cases, such as Quebec (Canada), chlorination of wastewater is not permitted (Ministère du Développement durable, de l'Environnement et de la Lutte contre les changements climatiques (MDDELCC), 2015).To reduce the chlorine concentration in the effluent, a dechlorination process is frequently required. Thus wastewater treatment plants are beginning to examine alternatives to chlorine disinfection; they include ultraviolet radiation (UV), ozonation and more recently developed alternatives, peracids.

## 2.2 Sodium hypochlorite

Sodium hypochlorite (NaOCl), more commonly known as bleach, is one of the most widely used methods of wastewater disinfection. Upon injection into the wastewater, the NaOCl decomposes to HOCl and some $OCl^-$, which ensure disinfection ("Sodium hypochlorite as a disinfectant", 2017).

NaOCl presents many advantages to alternatives: its use is cost-efficient, reliable and efficient. Furthermore, the storage and transportation of NaOCl are much safer than for the now lesser-used chlorine gas. NaOCl is usually delivered by truck or train in bulk, at a chlorine content of about 12.5%. When using sodium hypochlorite, special attention must be brought to the materials used to handle it, as NaOCl will react with metallic compounds (National Institute of Standards and Technology (NIST), 2017).

NaOCl use entails a residual concentration remains in the water, which insures continued disinfection after application. However, chlorine is toxic to aquatic life and forms harmful by-products (US EPA, 1999). To protect aquatic life, a dechlorination step is often added to the disinfection system (US EPA, 2000). Sulfur dioxide, sodium bisulfite and sodium metabisulfite are most commonly used for dechlorination. The additional step of dechlorination requires extra materials and a more complicated operation system, which can be a disadvantage associated with its use (NIST, 2017).

## 2.3 Toxicity of sodium hypochlorite

The toxicity of chlorine has been thoroughly investigated through the years: Reports dating back to the 1970s established both the toxicity of free and combined chlorine for aquatic life (Brungs, 1973). The toxicity of NaOCl, depends not on the original applied dose, but on the residual chlorine remaining in the effluent. The toxicity also depends on the type of chlorine residual: free or combined. The proportion of each type in water depends on factors such as pH, temperature, contact time, the amount of chlorine added and the ammonia content of the water. Studies have concluded that free chlorine is more toxic than chloramines (combined chlorine); therefore, toxicity is increased at low pHs, when free chlorine dominates (Du et al., 2017). EC50s (concentration creating an effect in 50% of organisms exposed to chemical) as low as 0.04 mg/L have been reported for free chlorine (US EPA, 1992)

Furthermore, disinfection with chlorine can lead to the formation in effluents of disinfection by-products (DBPs) such as trihalomethanes (THMs) and haloacetic acids (HAAs), especially at high contact times (Du et al., 2017). A higher amount of by-products has also been reported with increases of temperature, pH and the amount of reactive materials (El-Dib and Ali, 1995). It has been demonstrated that long-term exposure to disinfection by-products can lead to an increased risk of cancer (Richardson et al., 2007). Chlorination of reclaimed water leads to higher levels of DBPs than chlorination of drinking water. More specifically, chlorinated reclaimed water present higher toxicity, anti-estrogenic activity and cytotoxicity in the indicator organism *Daphnia Magna* (Ye Du et al., 2017).

Quenching is now used in many treatment plants still using chlorine for wastewater disinfection in order to protect aquatic organisms from chlorine. Removing chlorine also leads to a decrease in DBP formation (Du et al., 2017).

## 2.4 Peracetic acid

Peracetic acid (PAA, $CH_3CO_3H$) is a disinfectant that has been used in the food, beverage and medical industries for many years, however, for wastewater treatment it was first proposed in 1976 by Meyer in the Journal of Hygiene Epidemiology and Immunology (Luukkonen et al., 2015 ). The commercially available disinfectant is commonly an equilibrium mixture of peracetic acid (12 – 18%), hydrogen peroxide (18.5 – 23%), water (about 51%), and acetic acid (about 18%). The mechanism of disinfection with PAA occurs through the formation of highly oxidizing radicals. When using PAA, some measures must be taken to ensure a safe working environment as it is highly corrosive, and it is classified as a primary irritant and mutagen (Luukkonen et al. 2015).

PAA has many advantages compared to chlorine disinfection: It is safer to use, usually requires lower doses due to its high oxidation potential, and due to its rapid degradation, exposure of aquatic life to it is limited (Kitis, 2004, Luukkonen et al., 2015). Furthermore, the transition from chlorine disinfection to PAA for existing treatment plants is easily done; no major capital investment is necessary. The bulk of the cost of using PAA comes from the PAA itself; the cost per unit of disinfectant is higher than for chlorine based disinfectants, due to the limited worldwide production capacity (Kitis, 2004). A possible problem that can occur when PAA is used is a slight increase of organic matter in the effluent due to the acetic acid present in the PAA mixture and PAA decomposition, which could potentially cause microbial regrowth (Kitis, 2004).

Contact time for PAA disinfection of secondary effluents is up to 30 minutes at doses of 1 to 7 mg/L for a 3 log reduction in total coliforms. For biologically treated water, the dose can be 1.5-

2 mg/L with contact times of 10-15 minutes (Luukkonen, Teeriniemi, Prokkola, Rämö & Lassi, 2014). The dosing system typically includes tanks for PAA storage, dosing pumps, PAA diffusers and a residual monitoring system.

To date, three different PAA formulations, described in Table 1, have been approved by the EPA for use in the USA: VigorOX WWT II by PeroxyChem ("Wastewater Disinfection", 2017), Proxitane WW-12 by Solvay ("PROXITANE® | Solvay", 2017) and BioSide by EnviroTech ("Bioside HS 15% - Enviro Tech Chemical Services, Inc.", 2017). Over 20 treatment plants, in the USA and Canada, as well as many plants in Europe, use it for treatment (Santoro et al., 2017).

*Table 1. PAA formulations approved for use in the USA by the EPA*

| *Formulation* | *Provider* | *Contents* |
|---|---|---|
| *VigorOX WWT II*<br>*Source: Peroxychem* | PeroxyChem | 15% peracetic acid<br>23% hydrogen peroxide<br>45% water<br>16% acetic acid<br>1% sulfuric acid |
| *Proxitane WW-12*<br>*Source: Kelly Solutions* | Solvay | 12% peracetic acid<br>18.5% hydrogen peroxide<br>49.5% water<br>20% acetic acid |
| *BioSide*<br>*Source: Aquapulse Chemicals* | EnviroTech | 14-17% peracetic acid<br>21-23% hydrogen peroxide<br>40-51% water<br>14-20% acetic acid |

## 2.5 Performic acid

Performic acid (PFA, $CH_2O3$) is a wide-spectrum disinfectant recently available for wastewater treatment (Ragazzo, Chiucchini, Piccolo & Ostoich, 2013). Not yet used in North America; PFA is however becoming more common on Europe, with treatment plants in Italy, Denmark, Germany and France (Système d'Information sur l'Eau du Bassin Adour Garonne (SIEAG). 2017; Ragazzo et al., 2013; Chhetri et al., 2014; Ragazzo, Chiucchini, Piccolo & Ostoich, 2013).

Because of its unstable nature, PFA must be produced on-site, by combining hydrogen peroxide, formic acid and sulfuric acid. Also used for many years in fields other than wastewater treatment, such as medicine and the food industry, the first trials for wastewater disinfection with PFA were started in 2004 in two treatment plants near Venice, Italy (Ragazzo, Chiucchini, Piccolo & Ostoich, 2013). Because PFA use in wastewater treatment is so recent, much about its mode of action and toxicity remains unknown (Ragazzo et al., 2017). Safety concerns are important, as PFA becomes very unstable at high temperatures and concentrations (Luukkonen, Heyninck, Rämö & Lassi, 2015). Partly due to its higher oxidation potential, the required dose for disinfection is smaller than that for PAA. Furthermore, its rapid degradation to hydrogen peroxide and formic acid once in contact with influent ensures that the residual released into the environment by the treated effluent is much smaller (Karpova et al., 2013). Another advantage presented by PFA is the relatively low investment cost associated with its use, especially for large treatment plants as the disinfectant is produced on-site. However, the cost of PFA is still superior to that of chlorine (Chhetri et al., 2014). An automated mixing unit is typically provided containing all equipment needed for dosing such as storage tanks for chemicals and transfer pumps. Due to small doses, the entire unit requires little space at the treatment plant (Kemira, 2017), nevertheless the contact tank may be approximately the same size as that for chlorine or PAA. The concentration of performic acid in the solution used for wastewater treatment is typically between 8 and 15% by weight.

## 2.6 Toxicity of peracids

While more is known about the toxicity of PAA, only recently has the toxicity of PFA been investigated. Chhetri et al. (2017) compared the toxicity of PFA and PAA on the 72h growth rate inhibition of green microalgae *Pseudokirchneriella subcapitata.* Both acids presented clear toxicity and dose-response curves could be determined. These results, reported in Table 2, are considerably higher than those in previous reports of PAA toxicity.

Antonelli et al. (2009) investigated the toxicity of PAA using four indicator organisms: *Vibrio fischeri*, *Thamnocephalus platyurus*, *Daphnia magna* and *Selenastrum capricornutum*. The conclusion was that PAA was toxic for bacteria and crustaceans at concentrations lower than those used for wastewater disinfection, but that algae (*Selenastrum capricornutum*) were much less sensitive to PAA than the other test organisms (Table 2).

*Table 2. Reported $EC_{50}$s for PAA, PFA and $H_2O_2$*

| *Chemical* | *Test organism* | *Contact time* | *EC50 (mg/L)* | *Source study* |
|---|---|---|---|---|
| PAA | V. *fischeri* | 5 min | 0.087 | Antonelli et al. (2009) |
| | | 15 min | 0.102 | |
| | | 30 min | 0.131 | |
| | T. *platyurus* | 90 min | 0.049 | |
| | D. *magna* | 24h | 0.152 | |
| | S. *capricornutum* | 72h | 8.89 | |
| | P. *subcapitata* | 72h | 1.38 | Chhetri et al. (2017) |
| | V. *fischeri* | 15 min | 0.109 | Chhetri et al. (2014) |
| PFA | P. *subcapitata* | 72h | 0.340 | Chhetri et al. (2017) |
| | V. *fischeri* | 15 min | 0.376 | Chhetri et al. (2014) |
| $H_2O_2$ | P. *subcapitata* | 72h | 2.90 | Chhetri et al. (2017) |
| | V. *fischeri* | 15 min | 12.0 | Chhetri et al. (2014) |

$EC_{50}$ values are determined using the initial dose of peracid. When peracids are applied to effluents from WWTPs, they undergo decay kinetics; therefore, the exposure dose will decrease over the time of exposure. However, as stated by Antonelli et al. (2009), "any inhibition or adaptation effect of the test organism to PAA represents a response to the initial value of the disinfectant". Furthermore, it needs to be determined whether the toxic effect is a consequence of residual peracid, or if it is due to a reaction between peracids and other components in the effluents. For example, Guzella et al. (2004) observed that the toxic effects of PAA were more acute in effluents with high organic and suspended solids contents.

As mentioned, peracids quickly degrade to hydrogen peroxide. It is therefore important to consider the toxicity of hydrogen peroxide as well; this was investigated by Chhetri et al. (2014&2017). The toxicity of hydrogen peroxide was reported to be much lower (Table 2) than for PAA and PFA.

## 2.7 Life cycle assessment

In order to normalize the methodology used in life cycle assessment, the International Standards Organization (ISO) has published two standards, ISO 14040 (2006) and ISO 14044 (2006). These standards have set specific steps that must be followed for a complete and credible life cycle assessment and life cycle impact assessment. They also prevent project sponsors from manipulating studies in order to obtain favourable results.

A complete life cycle assessment consists of four essential steps:

### 2.7.1 Definition of the goal and scope

In the definition of the goal and scope of the LCA, the function of the product system investigated is determined as well as the functional unit and the boundaries of the systems. The intended public as well as the applications of the study are also decided. Other choices that are made at this point in the project include the allocation procedures, impact assessment methodology, interpretation methodology, data requirements and assumptions. Because LCA uses an iterative approach, these components can be modified further as the project proceeds if the need presents itself.

#### 2.7.1.1 Functional unit

Past LCAs applied to wastewater treatment have provided insight on the best choice of a functional unit when comparing different treatment methods. Defining a functional unit based only on volume treated, the most frequently used method in the past, does not take into account differences in influent and effluent quality (Corominas et al., 2013). For LCAs considering entire treatment plants, Zang et al. (2015) suggest the use of two functional units, one based on volume treated and another on eutrophication potential, i.e. $PO_4^{3-}$ removed. Tillman et al. (1998) suggest using one functional unit, based on population equivalent (PE) where 1 PE is defined as being the organic biodegradable load having a five-day biochemical oxygen demand ($BOD_5$) of 60 g of oxygen per day.

#### 2.7.1.2 System boundaries

Defining the boundaries for product systems in wastewater treatment presents a challenge and the choices made can have a major effect on the results of the LCA. The boundaries depend on many aspects of the LCA such as the goal and scope, applications and audience, assumptions, data constraints, etc. (ISO 14040, 2006). The following include some of the more important processes to consider when deciding on boundaries:

- Raw materials acquisition
- Inputs and outputs of manufacturing processes
- Transportation and distribution
- Energy and electricity sources
- Use and maintenance of products
- Recovery and reuse
- Manufacture of ancillary materials
- Manufacture, maintenance and decommissioning of capital equipment
- Other secondary operations such as lighting and heating

In their survey of past LCA studies applied to wastewater treatment, Corominas et al. (2013) grouped the studies reviewed according to the following figure.

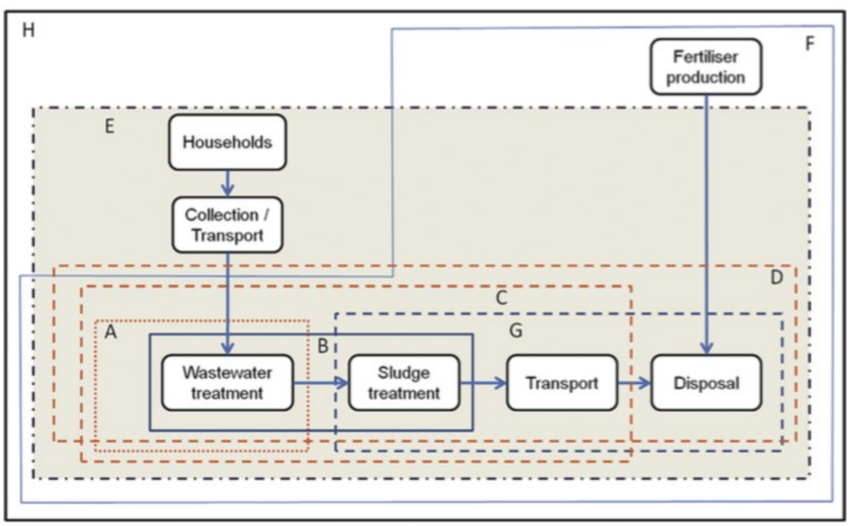



*Figure 1. System boundaries identified in review of wastewater LCAs*
*Source: Corominas et al. (2013)*

The distribution of boundaries used is summarized in the following table.

*Table 3. Distribution of boundaries shown in Figure 1*

| *Boundaries* | *# of studies* | *Description* |
|---|---|---|

| | | |
|---|---|---|
| *A* | 5 | Wastewater treatment process only |
| *B* | 4 | Wastewater and sludge treatment |
| *C* | 2 | Wastewater treatment, sludge treatment and transport |
| *D* | 14 | Wastewater treatment; sludge treatment, transport and disposal |
| *E* | 0 | Recovered energy from organic matter in toilet wastewater and household biowaste; wastewater treatment; sludge treatment, transport and disposal |
| *F* | 13 | Wastewater treatment; sludge treatment, transport and disposal; avoided fertiliser production |
| *G* | 1 | Sludge treatment, transport, and disposal |
| *H* | 8 | All processes described above |

*Source: Corominas et al. (2013)*

As the table indicates, most studies included wastewater treatment, sludge treatment as well as transport and disposal of the sludge. A large number of studies included the same boundaries, but added fertilizer production to the system.

As the figure demonstrates, there is high variability in the boundaries chosen for the LCAs. Of the 45 studies used to compare boundaries, 23 included only the operation of the treatment plant, and did not consider the construction and demolition phases. However, of the studies which did include construction and demolition, 6 found that these phases of the LCA did have an impact worth taking into account, whether the treatment system be very low-tech (wetlands and reedbeds), or high-tech (activated sludge systems and membrane bioreactors).

### 2.7.2 The inventory analysis

The inventory analysis entails the quantification of all the inputs and outputs of the product systems (International Standards Organization (ISO) 14040, 2006). Thee process is described graphically in Figure 2. First, all inputs and outputs relevant to the procedures included in the system boundaries are identified. Then, the quantities of inputs and outputs must be determined relative to the functional unit of the study. The inventory analysis is an iterative process: as data are collected, it is possible to discover limitations and it could be necessary to make certain assumptions. This can lead to a modification of the goal and scope in order to ensure coherence between the different LCA stages.

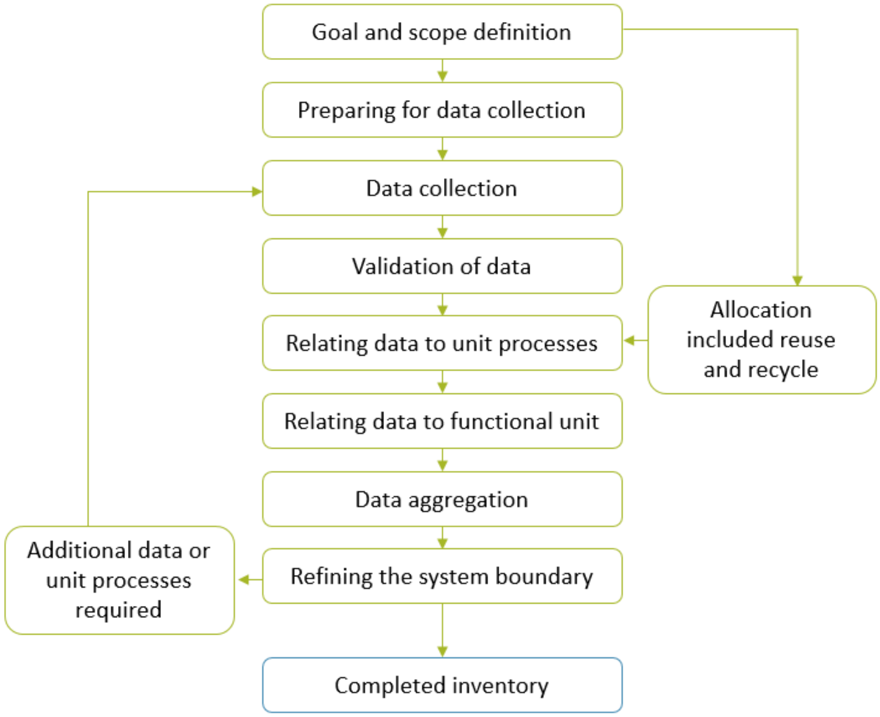



*Figure 2. Simplified procedures for inventory analysis*
*Source: ISO 14044 (2006)*

Sources of data are varied. In order to help LCA practitioners, different databases containing background processes have been developed over the years. At present, the database with the largest quantity of high quality data is the ecoinvent database, developed in Switzerland. It currently contains information on more than 12 800 processes (Ecoinvent.org, 2017). The database is updated regularly and it links data to specific geographical locations. It is claimed that using such a database ensures that the data used are consistent, up to date and reliable. Furthermore, when using the database it is possible to edit information in order to have a more accurate representation of reality if processes differ slightly.

When information needed is not contained in a database, other sources must be considered: On-site measurements, design documents and vendor-supplier information can also be used (Corominas et al. 2013).

The primary source of data for LCA applied to wastewater treatment are the treatment plants themselves. When data from WWTPs are not available, the secondary source of data is usually pilot studies and bench scale experiments. Background information can be taken from free or licensed LCI databases such as ecoinvent (Ecoinvent.org, 2017), GaBi (Gabi-software.com, 2017), European Life Cycle Data (European Platform on Life Cycle Assessment, 2017), the U.S. Life Cycle Inventory Database (National Renewable Energy Laboratory (NREL), 2017) as well as many others.

### 2.7.3 The impact assessment

Once the emissions of the system have been quantified, the impact assessment will determine where and in which quantity the emissions will have the most effect. To do this, impact categories, category indicators and characterization models are selected. A midpoint characterization aggregates the emissions into midpoint impact categories, which represent different environmental problems such as human toxicity, ozone layer depletion or eutrophication, among others. Then, the midpoint categories can be combined to form endpoints or damage categories such as human health, ecosystem quality, resource consumption or climate change. The choice of whether to aggregate the midpoints into endpoints is left to the user. The main steps of the LCIA are described below.

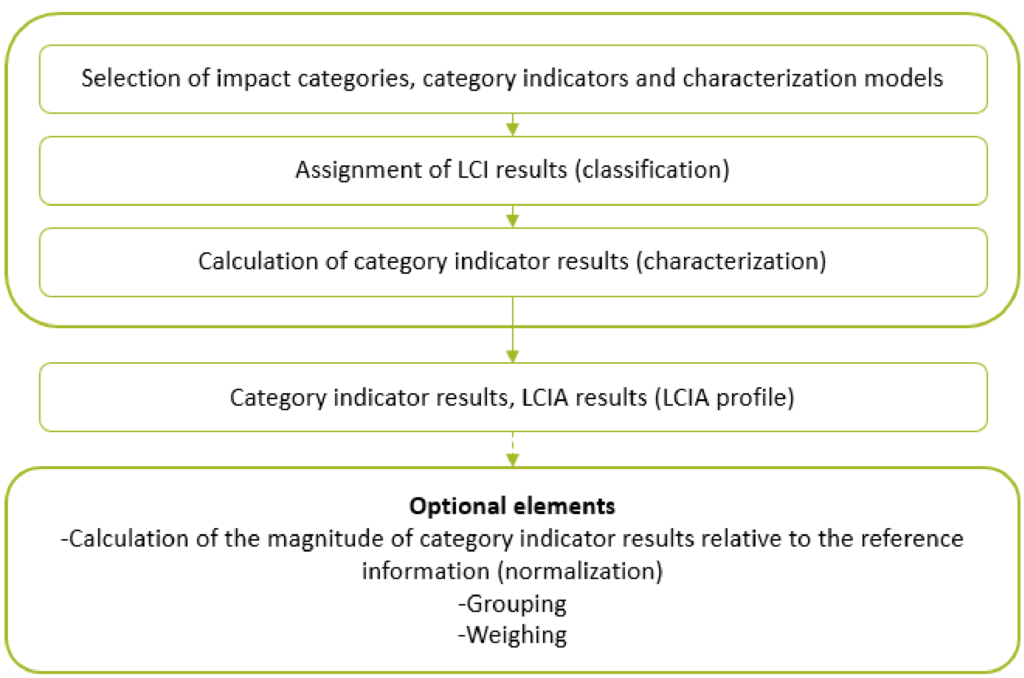



*Figure 3. Elements of the LCIA phase*
*Source: ISO 14044 (2006)*

Aggregating results into endpoints can make the decision-making process much easier as it is easier to interpret the results and the environmental relevance increases; however staying at the midpoint level reduces the uncertainty of the study (Hauschild, Rosenbaum and Olsen, 2017).

In order to bring uniformity in the life cycle impact assessment, various characterization models have been developed. The choice of the model to use depends greatly on the goal and the scope of the LCA.

According to the review of LCA applied to wastewater treatment done by Corominas et al. (2013), the most widely used impact assessment method is CML (Guinée, 2006). Other popular impact assessment methods include EDIP97 (Wenzel, Hauschild and Alting, 1997), Eco-indicator 99 (Goedkoop and Spriensma, 2001) as well as Impact 2002+ (Jolliet et al., 2003). Renou et al. (2008) investigated whether the choice of the impact assessment method can influence results in LCAs applied to wastewater treatment and found that indeed, the choice of the model can influence results, but not for all impact categories. For global warming, acidification, eutrophication and resource depletion, all investigated models yield similar results. However, the results obtained for human toxicity and ecotoxicity can be very different from one model to another (Hauschild et al., 2017)

The most popular impact categories for LCA applied to wastewater treatment include global warming potential, acidification and eutrophication (Corominas et al., 2013). Other impact categories often considered are photochemical oxidation, human and eco-toxicity, ozone depletion and abiotic resources depletion.

It is also worth mentioning that the impacts calculated from an LCA study are only potential future impacts. They are expressed in reference to the functional unit and are therefore not a prediction of actual effects of a product system. The potential impacts are based on inventory data that are integrated over time and space, and therefore occur on different time horizons and different locations (Hauschild et al., 2017).

#### 2.7.3.1 The USEtox model

For potential toxicity impacts, the scientific consensus is that the USEtox method provides the most accurate results. Developed by the United Nations Environment Program and the Society for Environmental Toxicology and Chemistry, "USEtox represents best application practice as an interface between ever advancing science and a need for stability, parsimony, transparency, and reliability" (usetox.org, 2017). USEtox relies on both the midpoint and the endpoint approaches. The midpoints of the USEtox model are freshwater ecotoxicity, human cancer affects and human non-cancer effects. The model then aggregates the midpoints into two endpoint categories: ecosystem toxicity and human toxicity.

The impact pathways that USEtox relies on are shown in Figure 4.

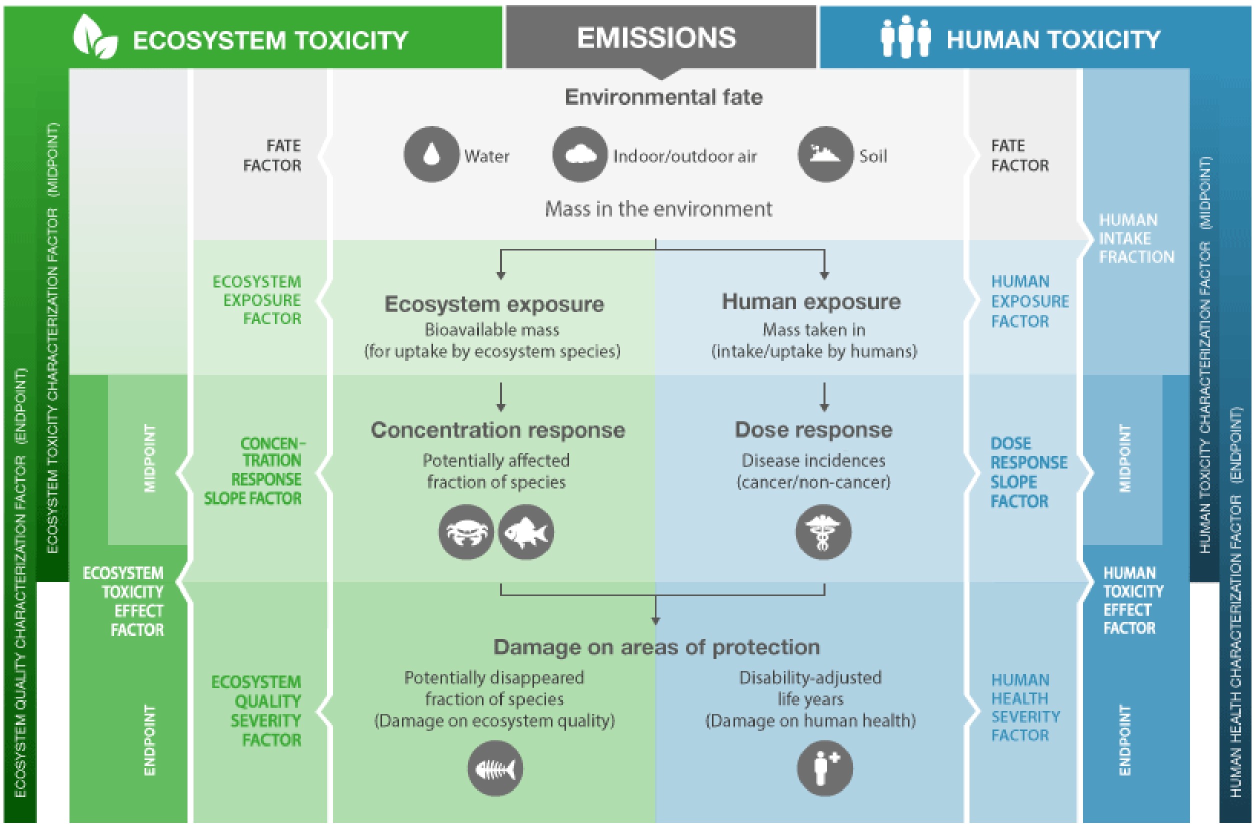



*Figure 4. USEtox comparative toxicity assessment framework*
*Source: usetox.org*

The model works at different scales such as indoor, outdoor, continental and global environments, which are then divided into several compartments, illustrated in Figure 5.

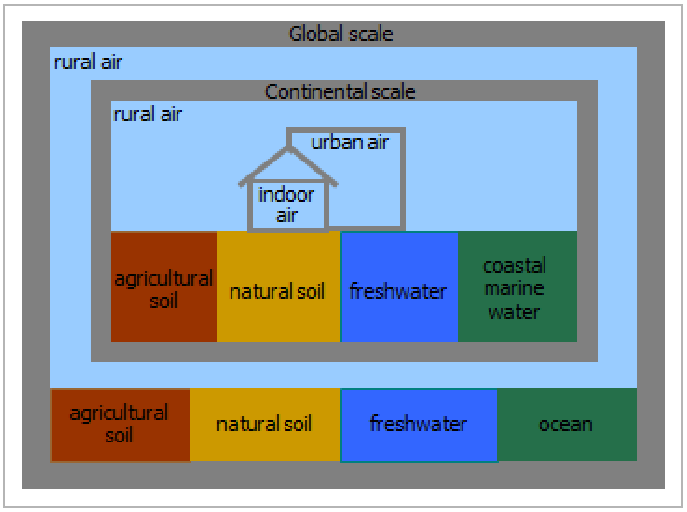



*Figure 5. USEtox environmental compartment structure*
*Source: usetox.org*

The outputs of the USEtox model are characterisation factors, used to determine the potential toxicity impact per kg of substance released into the environment. The characterisation factors for aquatic toxicity and human health are developed using three components: Environmental fate, exposure and effect. The environmental fate factor provides insight on how the substance released is distributed into the environment and how it degrades. The exposure factor determines the exposure of humans, animals and plants and the effect will express how much damage will ensue from exposure. For the freshwater ecotoxicity midpoint, the characterisation factor calculated is expressed as potentially affected fraction of species integrated over time and volume. The characterisation factor for human health midpoint is expressed as disease cases per kg emitted. The characterisation factor is then multiplied by the mass of substance released into the environment for each product system compared.

A unique advantage in using the USEtox model is the large number of characterisation factors developed for human and aquatic toxicity. While LCA studies could include thousands of different chemical substances, the current models contain the characterisation factors for only a fraction of them (usetox.org). The USEtox model contains the highest number and is the recommended model for the abovementioned midpoint categories.

The USEtox model is also unique because it provides the methodology for calculating new characterisation factors. This allows LCA practitioners to calculate characterisation factors for substances that are not yet included in the database. These new characterisation factors are qualified as "interim characterisation factors" because they have not gone through the extensive scientific review process used for characterisation factors included in the database, "recommended characterisation factors". Interim characterisation factors are often calculated for metals or non-organic substances, which can dominate the overall potential impacts of the product systems (Golsteijn, 2014). The uncertainty of interim factors is very high; the results of a study with interim characterisation factors should be interpreted very carefully, and sensitivity analysis should be used in order to investigate how the results are affected by the interim characterisation factors.

2.7.3.2 Impact 2002+ model

The impact 2002+ model also relies on both the midpoint and the endpoint approach, where the LCI results with similar impact pathways are allocated to impact categories at the midpoint level. The model then aggregates the midpoints into endpoints, included in Table 4. The newest version of Impact 2002+ has updated its methodology, and has transferred or adapted methods from other popular impact assessment methods such as Eco-indicator 99 and CML 2002, among others (Humbert et al., 2012).

*Table 4. Endpoints and midpoints of the Impact 2002+ characterization model*

| *Endpoint categories/Damages and units* | *Midpoint category/Problems* | *Midpoint unit* | *Model Uncertainty at midpoint level* |
|---|---|---|---|
| *Human health (DALY)* | Human toxicity | kg chloroethylene in air –eq. | High |
| | Respiratory effects | kg $PM_{2.5}$ in air –eq. | Low |
| | Ionizing radiation | Bq Carbon-14 into air –eq. | High |
| | Ozone layer depletion | kg CFC-11 into air –eq. | Medium |
| | Photochemical oxidation | kg ethylene into air –eq. | Medium |
| | Aquatic toxicity | kg Triethylene glycol into water –eq | High |
| *Ecosystem quality ($PDF \cdot m^2 \cdot y$)* | Terrestrial ecotoxicity | kg Triethylene glycol into soil –eq | Very high |
| | Aquatic acidification | kg $SO_2$ into air –eq | Low |
| | Aquatic eutrophication | kg $PO_4^{3-}$ into water –eq | Low |

| | | | |
|---|---|---|---|
| | Terrestrial acidification | kg $SO_2$ into air –eq | High |
| | Land use | $m^2$ Organic arable land –eq·y | High |
| | Water turbined | inventory in $m^3$ | Low |
| *Climate change (kg eq. $CO_2$)* | Global warming | kg $CO_2$ into air –eq. | Low |
| *Resources (MJ)* | Non-renewable energy | MJ or kg Crude oil –eq (860 kg/$m^3$) | Low |
| | Mineral extraction | MJ or kg Iron-eq (in ore) | Medium |

*Source : Humbert et al., 2012*

Only the climate change and resources midpoints will be used for the current LCA. Impact 2002+ considers global warming potential for a 100-year time horizon. The model considers emissions to air only for climate change: $CO_2$, fossil, from land transformation and biogenic; CO, fossil and biogenic; $CH_4$ fossil and biogenic. Only the direct effects of $CH_4$ are considered, not the effects of $CO_2$ once the $CH_4$ has degraded to $CO_2$.

The resource midpoints include non-renewable energy and mineral extraction. Non-renewable energy is calculated using upper heating values and is expressed in MJ total primary non-renewable energy per unit extracted (Humbert et al., 2012). Mineral extraction is also expressed in MJ/unit extracted, based "on the assumption that extraction leads to an additional energy requirement for further mining of this resource in the future, caused by lower resource concentrations or other unfavourable characteristics of the remaining reserves" (Jolliet et al., 2003).

### 2.7.4 Interpretation of results

In the final step of the LCA, the results obtained through the impact assessment are identified, qualified and evaluated. Uncertainties linked to the study are examined and if necessary, sensitivity analysis helps to determine whether the uncertainties have an important impact on results of the LCA. The interpretation must include an analysis on how the choices made throughout the study (assumptions, models and impact categories selected, data used) affect the results (Jolliet et al., 2016). Depending on the goal of the LCA, within the same product system, the contribution of the different life cycle phases can be investigated, and different product systems should be compared based on their environmental performance. Special attention should be brought to the presentation of results in order to ensure that they do not lead to bias during the interpretation, and the analysis should take into account whether results from the study are made public.

# 3. Study design

## 3.1 Goal

The general objective of the study is to compare the use of three different wastewater disinfection products: sodium hypochlorite, peracetic acid and performic acid. More specifically, the objectives are the following:

1. Evaluate which product has the highest potential impact on freshwater toxicity, climate change, human toxicity, mineral extraction and non-renewable energy depletion;
2. Determine which life cycle stages of each product system have the highest potential impact;

The treatment plants used for the study are a treatment plant located near Venice, Italy, and the Northwest Langley treatment plant near Vancouver, Canada.

## 3.2 Scope

### 3.2.1 Location of the study

Life cycle assessment applied to wastewater treatment is case specific as no two wastewater treatment plants are identical (Stokes & Horvath, 2010). The main difference lies in the influent water quality, which varies as a function of type and size of population served, country, seasons, etc. Furthermore, treatment processes differ greatly due to regulation, available treatment options, budgets, and other factors. This means that the results of LCAs are not easily transferrable to other treatment plants, which must be specified in the goal and scope definition. Nevertheless, the results of a comparative analysis can provide an indication of the relative merits or demerits (in the context of LCA), especially if there are major differences.

The two locations used for the study are the following:

3.2.1.1 Venice-area Wastewater Treatment Plant, Italy

The Venice-area treatment plant serves a municipality of 26 000 residents, however, the area served is a resort city and therefore larger seasonal variations in the amount of wastewater treated are observed due to a high influx of tourists in the summer months. The area includes a few small industries such as car washes, laundry facilities and similar services. The treatment plant is therefore designed to serve a population equivalent of 160 000 and the daily flows varies between 16 and 44 MLD. A conventional sequence of sewage treatment, including primary clarification, activated sludge, secondary settling and disinfection is used at the treatment plant. The final effluent is discharged into the Adriatic Sea (Ragazzo, Chiucchini, Piccolo & Ostoich, 2013).

The treatment plant traditionally uses NaOCl for disinfection. Many trials with alternative disinfectants have been done there, starting with PAA in 2006. In 2012, the performance of PFA was investigated in partnership with Kemira Oyj, who provided the DesinFix unit, which produces PFA on-site by mixing formic acid with hydrogen peroxide.

The 2006 trials with PAA determined that a dose between 0.9 and 2.1 mg/L and a retention time of 16 minutes was sufficient to achieve effluent concentrations of E. *coli* below the required limit of 5000 CFU. With PFA in 2012, the dose required was between 0.6 and 1.4 mg/L with a retention time of about 18 minutes.

3.2.1.2 Northwest Langley Treatment Plant, British Columbia, Canada

The Northwest Langley Treatment Plant, managed by Metro Vancouver, treats an average flow of 11.5 MLD and serves a population of about 27 000 residents, and no industries. It uses a trickling filter and activated sludge for secondary treatment, and has no primary treatment. The treatment plant was designed to nitrify but does no denitrification. Disinfection only occurs from the months of April to October at NW Langley, and the effluent is discharged into the Fraser River. Before 2012, the treatment plant treated the secondary effluent using sodium hypochlorite (NaOCl, 12% solution), and used sodium bisulfite ( 38% solution) for dechlorination, due to Canadian regulations stating that the chlorine residual could not surpass 0.1 mg/L (Goldman et al., 2016).

In 2015, regulations changed and the chlorine residual allowed in the effluent decreased to 0.02 mg/L. This, added to the fact that nitrification increased the chlorine demand at the treatment, motivated Metro Vancouver to investigate alternatives to NaOCl disinfection (Goldman et al., 2016).

Regulations for the NW Langley effluent state that the 30-day geometric mean for fecal coliforms must be less than or equal to 200 MPN/100 mL at the edge of the dilution zone (IDZ). The dilution ratio at the IDZ is 51:1. This translates to a 30-day geometric mean of less than 10 200 MPN/100 mL. Regulations also control the amount of carbonaceous biochemical oxygen demand (cBOD), total suspended solids (TSS), and un-ionized ammonia (Goldman et al., 2016).

In 2012, a pilot test was done to determine whether it would be feasible for the treatment plant to transition to PAA disinfection. PAA was chosen as a disinfectant for many reasons: ease of implementation, low capital investment and the fact that quenching would not be needed. The pilot test revealed that the disinfection target could easily be achieved using PAA with a formulation of 21%. Furthermore, no increase in cBOD was observed in the effluent. Following the pilot tests, PAA disinfection was fully implemented in 2013. Initial tests indicated that a dose of 2.5 mg/L of PAA was needed in order to meet regulations on *E. coli* and fecal coliforms. The required dose for sodium hypochlorite disinfection had been 2.6 mg/L, therefore the doses of PAA and NaOCl were similar (Goldman et al., 2016).

Toxicity tests were also done at the treatment plant on both formulations of PAA available in Canada: Proxitane WW-12 and VigorOx WWT II. The $LC_{50}$ 96 hours residual concentrations determined were 4.2 mg/L for Proxitane and 3.5 mg/L for VigorOx. The required dose at NW Langley being 2.5 mg/L and the demand being of 1.7 mg/L, the residual concentration of PAA is well below the toxicity threshold (Goldman et al., 2016).

### 3.2.2 Function

The function of the product systems is to disinfect wastewater before releasing the effluent into the environment.

### 3.2.3 Functional unit

Two treatment plants are studied for the LCA, the first being located in Venice, Italy (PAA, PFA and NaOCl used) and the second near Vancouver, Canada (PAA and NaOCl only). Because the flow, wastewater composition and processes differ in both treatment plants, the two treatment plants will be treated as two separate LCAs. Due to different practices and regulations in Italy and Canada, the functional unit will also differ for both treatment plants.

#### 3.2.3.1 Venice WWTP

The functional unit for the study is the removal of 3 log of E. *coli* at a municipal WWTP with a flow of 27 MLD located in Venice, Italy, following secondary treatment during the months of August and September.

#### 3.2.3.2 NW Langley WWTP

The functional unit for the study is the disinfection of the NW Langley WWTP effluent to a concentration of less than 200 MPN/100 mL fecal coliforms at the edge of the initial dilution zone, at a flow of 11.5 MLD, during the disinfection season from April 1$^{st}$ to October 31$^{st}$.

### 3.2.4 System boundaries

#### 3.2.4.1 Venice WWTP

Three scenarios are compared at the Venice WWTP. The process tree is included in Figure 6; each process is fully described in Section 4.3. Included in the LCA are the production and transport of the disinfectants, the production and transport of the storage containers for the chemicals, the raw materials needed for the production of the contact tank, the disinfection process itself as well as the residuals released to the environment at the end of the disinfection process.

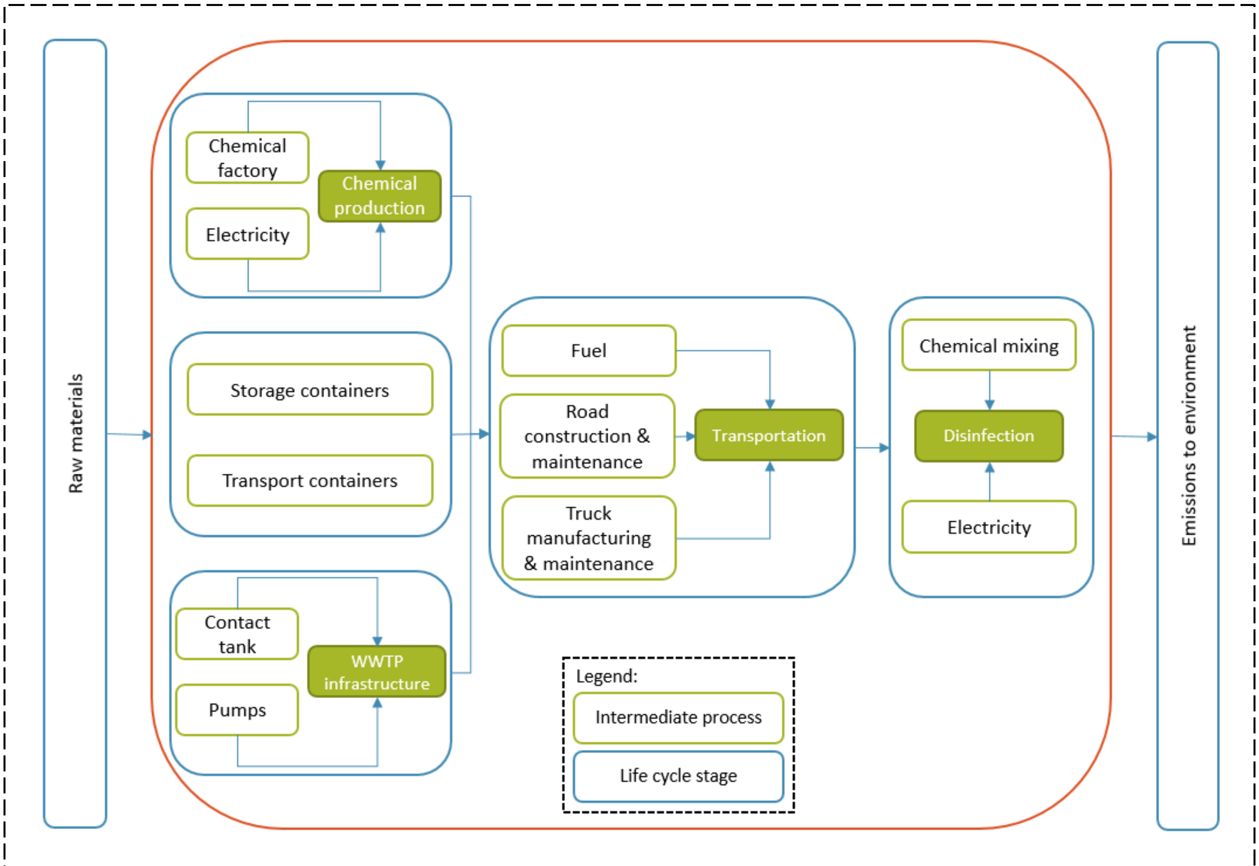



*Figure 6. Life cycle boundaries for the Venice WWTP*

3.2.4.2 NW Langley WWTP

The system boundaries, shown in Figure 7, for the NW Langley treatment plant are identical to the Venice plant in all regards but one. Whereas there was no further treatment at the Venice plant following disinfection, the NW Langley plant dechlorinated the effluent, using sodium bisulfite, to concentrations of chlorine below 0.1 mg/L, due to Canadian regulations. Therefore, the NW Langley treatment plant contains the additional processes of sodium bisulfite production, transportation of chemicals as well the dechlorination process itself. The residual sodium bisulfite was also added to the LCA. Furthermore, the NW Langley treatment plant only compares the use of NaOCl and PAA. A more detailed description is included in Section 4.3.

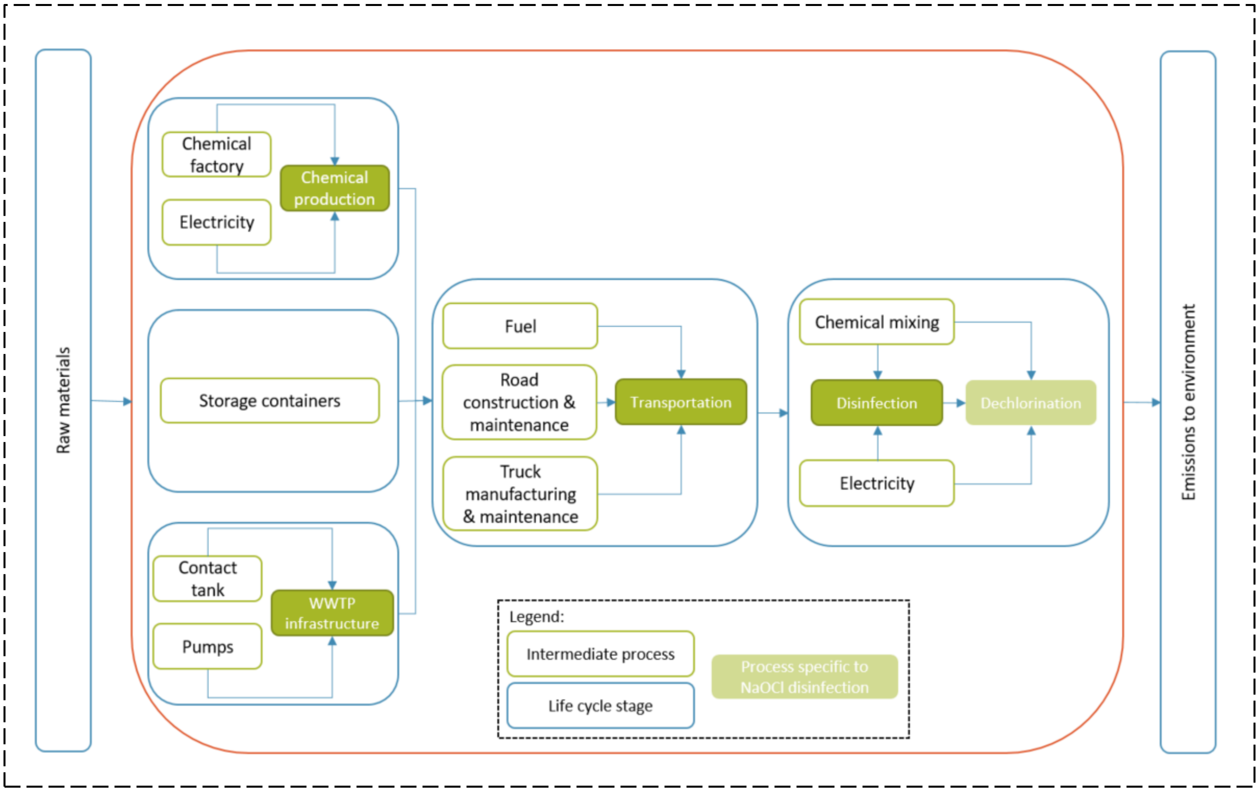



*Figure 7. Life cycle boundaries for the NW Langley WWTP*

### 3.2.5 Impact categories and impact assessment methodology

Whereas past LCA studies focused on wastewater treatment at the level of secondary treatment, the current LCA had the objective of determining which disinfection product, considered as a tertiary treatment process, has the lowest potential environmental impact. Following disinfection, the effluent containing residuals from chemical disinfection is released into the environment. Therefore, the potential impact on freshwater ecotoxicity for each chemical is very important for the LCA.

The USEtox model has characterisation factors for freshwater ecotoxicity and human toxicity midpoints. The units for each midpoint are further described in Table 6. A major strength of the USEtox model is that it contains many such characterisation factors, and therefore considers chemicals that other impact models fail to take into account. Hence, the USEtox model was chosen for this study. As mentioned earlier, LCAs can include thousands of different substances (Usetox.org, 2017). No model has developed recommended characterisation factors for all chemicals; there were therefore characterisation factors missing for elementary flows (i.e. the residuals) into the environment, illustrated as interim characterisation factors in Table 5. In order to determine the missing (interim) characterisation factors, the method published by USEtox for their calculation was used. Specific data used for the calculations are in Appendix E.

*Table 5. Recommended and interim characterisation factors on freshwater ecotoxicity for residuals from disinfection*

| *Disinfectants* | *Residuals* | *Characterisation factor* | *USEtox characterisation factor* |
|---|---|---|---|
| *NaOCl* | Free chlorine | Interim | 109 046 PAF*m$^2$*d/kg |
| | Combined chlorine | Recommended | 71 953 PAF*m$^2$*d/kg |
| | Sulfate | Interim | 62 PAF*m$^2$*d/kg |
| *PAA* | Peracetic acid | Interim | 11 865 PAF*m$^2$*d/kg |
| | Acetic acid | Interim | 49.831 PAF*m$^2$*d/kg |
| | Hydrogen peroxide | Recommended | - |
| | Sulfuric acid | Interim | 299.29 PAF*m$^2$*d/kg |
| *PFA* | Performic acid | Recommended | 48 920 PAF*m$^2$*d/kg |
| | Formic acid | Interim | 44.398 PAF*m$^2$*d/kg |
| | Hydrogen peroxide | Recommended | - |
| | Sulfuric acid | Interim | 299.29 PAF*m$^2$*d/kg |

The USEtox model contains characterisation factors for freshwater ecotoxicity for seven of the nine residuals present in the treatment plant effluents. The calculated characterisation factors are qualified as interim characterisation factors as they have not been validated by the scientific community and their uncertainty is very high. Nevertheless, the methodology strongly recommends using them, as the results of the study are compromised if they are not included.

Freshwater ecotoxicity is an important part of the LCA due to the chemical residuals being released into the environment; however, other midpoint categories were also used to compare the three product systems: Human toxicity, climate change and resource consumption. USEtox was used to model human toxicity (total of cancer and non-cancer effects) for the same reasons as freshwater toxicity. However, it was not possible to calculate interim characterisation factors for human toxicity as too little is known about the behaviour of substances for which characterisation factors were missing. The USEtox model calculates the potential impact on human toxicity by the uptake of chemicals into humans via different exposure pathways; therefore, the procedure is the same as for freshwater toxicity: characterisation factors developed through the model are based on a fate factor, an exposure factor and an effect factor.

The model used for climate change and resource consumption impacts was the Impact 2002+ model. The Impact 2002+ model also considers potential impacts on ecotoxicity and human health, however, it does not include as many characterisation factors as USEtox, nor does it provide a methodology to develop interim characterisation factors. Using the Impact 2002+ model, the potential impact on resource consumption, which includes non-renewable energy and mineral extraction was determined, as well as the potential impact on climate change.

*Table 6. Units for the midpoints of the USEtox and Impact 2002+ models*

| *Model* | *Midpoint* | *Units* | |
|---|---|---|---|
| *USEtox* | Freshwater toxicity | PAF*m$^2$*d/kg | Potentially affected fraction of species integrated over time and volume per kg emitted |
| *Impact 2002+* | Human toxicity | DALY/kg | Disease cases per kg emitted |
| | Climate change | kg $CO_{2eq}$ | Equivalent amount of $CO_2$ |
| | Non-renewable energy | MJ | Mega Joules |
| | Mineral extraction | MJ | Mega Joules |

*Sources : Usetox.org, 2017, Humbert et al., 2012*

# 4. Inventory analysis

## 4.1 Sources and methodology for data collection

The primary source of data for the LCA was the wastewater treatment plants being investigated. Published annual reports were used first, and to complete the inventory analysis questionnaires were sent to both treatment plants, Venice and Vancouver, in order to obtain additional information. Data from the NW Langley WWTP was provided by Metro Vancouver, a partnership of municipalities in the general Vancouver area that collaboratively plan and deliver regional-scale service (Metro Vancouver, 2017). Information about the Venice treatment plant was from ASI SpA, the firm responsible for the operation of the Venice WWTP. When information could not be provided from the primary sources, manufacturers were contacted directly for information. If neither the treatment plant, nor the manufacturers could provide the needed information, generic and theoretical data from a database or published literature were used.

The database used for the study was the ecoinvent database, built specifically to provide LCA practitioners with background information typically needed for LCAs. It is based in Switzerland. The APOS or Allocation at the Point of Substitution model, within ecoinvent, is used. This means that all inputs and outputs are linked to corresponding market activities. Furthermore, all materials for treatment are considered as "negative inputs" and multi output activities are allocated.

## 4.2 Desired quality of data

To compare the different disinfectants, all conditions needed to be as similar as possible to avoid interference from factors other than the type of chemical used for disinfection. The requirements for data quality from the two treatment plants were the following: The data had to be from the same months of the same year. Furthermore, only full-scale data would be considered in order to ensure the data were representative of full-scale and long-term treatment.

Lastly, the age of data had to be considered. Full-scale trials with PFA have been done very rarely and therefore, the age of the data could not be too restrictive. Data less than 10 years old were prioritized, but older data could not be completely excluded from the study.

## 4.3 Product system description and hypothesis

The main sources of data used for the study as well as the major hypothesises are described for each treatment plant in Table 7 to Table 9.

### 4.3.1 Equipment production

The equipment considered for the three product systems is quite similar. Included are the pumps, chemical containers and the contact tank where mixing occurs. Chemical containers for both transportation and on-site storage were considered. For PAA and PFA, high-density polyethylene (HDPE) containers of various sizes were used. NaOCl can be stored in both HDPE and fiber reinforces plastic (FRP), although studies indicate that FRP is the safest and best long-term option (Powellfab, 2017). For the study, FRP storage containers were therefore considered.

Because PFA is produced on-site, the DesinFix unit by Kemira Oyj was used for the LCA. The DesinFix unit consists of a steel cabinet, which contains all necessary equipment for the mixing and dosing of PFA: Pump, chemical containers and a mixing and cooling reactor. The treatment plants could not provide sufficient information on the tubing used to deliver the chemicals, therefore they were not considered.

*Table 7. Data on equipment used for disinfection at the Venice and the NW Langley WWTPs*

| *Reference flow* | *Key parameters* | |
|---|---|---|
| *Storage tank (PAA)* | Lifespan<br>Volume<br>Quantity | 5 years<br>29 526 L<br>1 |
| *Storage tank (NaOCl)* | Lifespan<br>Volume<br>Quantity | 5 years<br>2000 imp. gallons<br>1 |
| *DesinFix unit (PFA)* | Lifespan<br>Quantity | 10 years<br>1 |
| *Contact tank (Venice)* | Lifespan<br>Amount of concrete<br>Amount of steel | 30 years<br>53.45 $m^3$<br>1668 kg |
| *Contact tank (NW Langley)* | Lifespan<br>Amount of concrete<br>Amount of steel | 30 years<br>56.33 $m^3$<br>1758 kg |

### 4.3.2 Transportation

The transportation of the chemicals and their storage containers were considered for the study. All chemicals are considered to come from the same chemical factory, theoretically located 1 000 km from the treatment plants. It is also assumed the chemical containers come from the same factory as the chemicals. The chemicals and containers were assumed to be transported by truck capable of carrying 16-32 metric tonnes. The study takes into account emissions from transportation, truck manufacturing and maintenance as well as road construction and maintenance.

### 4.3.3 Electricity

Only the electricity directly used for disinfection was considered, therefore the amount of electricity used is quite low as it is only used for pump operation as well as the DesinFix unit operation for PFA treatment at the Venice WWTP. The DesinFix unit contains a cooling unit, which makes the total consumption of the product system higher than for NaOCl and PAA. The energy needed for lighting, temperature control (NaOCl requires storage at approximately 15°C for increased chemical stability) and other building requirements was not considered due to the unavailability of data. The location of the LCA was taken into account and the electricity grid used for the two locations is different. The sources of electricity for both Italy and British Columbia are described in Appendix A.

For electricity production and transmission, included are the electricity inputs from the country and the imports, transformed into medium voltage, the transmission network, the direct emissions to air and the electricity losses during transmission.

### 4.3.4 Chemical dosing and residual

Information on dose and residual was supplied by the treatment plants. At the Venice treatment plant, NaOCl and PFA disinfection achieved removals of 3 log on average. However, removal with PAA was lower; only 2 log removal was obtained. This was problematic as the functional unit was defined as removing 3 log of E. coli at the treatment plant.

To calculate the dose of PAA needed to obtain 3 log removal of *E. coli* at the Venice treatment plant, information in the kinetics of disinfection with PAA was supplied by the plant. Using the results of bench scale experiments and the double exponential model (Santoro et al., 2015), the necessary dose was calculated, as well as the residual from the modified dose. The residual obtained was for the active substance; no information could be obtained on the residuals of the other ingredients of the solutions such as hydrogen peroxide, acetic acid and formic acid as these are not tested for at the treatment plants. Regulations specify that *E. coli* concentrations in the effluent released from WWTPs in Italy must be below 5 000 CFU, however disinfection at the treatment plant in the years studied over-disinfected, achieving effluent concentrations in the 2 log range.

At the Northwest Langley treatment plant, information on the dose and residuals was obtained from full-scale trials done at the plant in 2012 and 2013 (Goldman et al., 2016).

*Table 8. Average dose and residual for the Venice and the NW Langley WWTPs*

| *Treatment plant* | *Disinfectant* | *Dose* | *Residual* |
|---|---|---|---|
| *Venice WWTP* | NaOCl | 2.79 mg/L | 0.62 mg/L combined chlorine<br>0.09 mg/L free chlorine |
| | PAA | 2.35 mg/L | 0.64 mg/L |
| | PFA | 0.91 mg/L | 0.16 mg/L |
| *NW Langley WWTP* | NaOCl | 2.6 mg/L | 0.7 mg/L total chlorine<br><0.1 mg/L after dechlorination (assumed 0) |
| | PAA | 2.5 mg/L | 0.80 mg/L |
| | $NaHSO_3$ | 4.71 mg/L | 2.34 mg/L as $SO_2$ |

Furthermore, not included in the residuals are the disinfection by-products such as trihalomethanes (THMs). Information on the type and quantities of disinfection by-products could not be provided by the treatment plants.

### 4.3.5 Chemical production

The inputs for the production of the 10% NaOCl solution were calculated using two different methods published by Forceflow Monitoring Systems (Forceflow.com, n.d.) and the Occidental Petroleum Corporation (Oxy.com, n.d.); these values were compared to the inputs of the NaOCl production flow in the ecoinvent database. The values obtained using the two published methods were the same however, the ecoinvent values were very different and did not include chlorine gas. The values calculated from the published methods were therefore used. Quantities for the production of 15% PAA were supplied by Peroxychem, and the quantities for the 13.6% PFA formulation were obtained directly from the Venice WWTP. The formulations and production process descriptions are included in Table 9. Production processes are allocated according to global market shares.

*Table 9. Inputs for the production of 1 kg of NaOCl, PAA and PFA solutions*

| *Inputs for 1 kg of disinfectant or solution* | | | *Process* |
|---|---|---|---|
| *NaOCl 10% solution* | Heat | 1.61 MJ | For steam production, quantities from ecoinvent database |
| | Sodium hydroxide | 0.153 kg | Chlor-alkali process: Electrolysis of a salt solution using three different technologies: Mercury (17.23% of production), diaphragm (42.8%) and membrane cell (40%) electrolysis |
| | Chlorine gas | 0.128 kg | Chlor-alkali process: Electrolysis of a salt solution using three different technologies: Mercury (45.8% of production), diaphragm (13.9%), membrane cell (39.9%) and sodium chloride electrolysis (0.37%) |
| *PAA 15% solution* | Acetic acid | 0.278 kg | Mosanto process: Carbon monoxide reacts with methanol under the influence of rhodium complex catalyst at 180°C and 3-4 MPa. |
| | Hydrogen peroxide | 0.297 kg | Autooxidation or Anthraquinone process: Produced by reducing alkylanthraquinone with hydrogen in the presence of a catalyst to the hydrochinone. |
| | Sulfuric acid | 0.007 kg | Contact process: $SO_2$ raw gases are oxidised to $SO_3$ on catalysts containing alkali and vanadium oxides, at temperatures between 420°C to 630°C. The SO3 obtained is absorbed in absorbers by concentrated sulfuric acid. In these absorbers, the $SO_3$ is converted to sulfuric acid by the existing water in the absorber acid. This acid is kept at the desired concentration by adding water or diluted sulfuric acid. |
| *PFA – 100%* | Formic acid | 2.512 kg | Decarboxylative cyclization of adipic acid (0.6% of production), methyl formate route (97.3%) and oxidation of butane (2.1%) |
| | Hydrogen peroxide | 3.490 kg | See above |
| | Sulfuric acid | 0.471 kg | See above |
| *Chemical factory* | | 1E-4 factory /kg | Infrastructure assessed using data from the chemical plant sites in Gendorf, Germany, and from the BASF site of Ludwigshafen, Germany. The factory is assumed to have a lifespan of 50 years and produces 50 000 tons/year. |

*Source: Chudacoff (2007), Hischier (2007), Althaus (2007), Ossés (2007), Sutter (2007)*

## 4.4 Results of the inventory analysis

Due to the extensive amount of data resulting from the inventory analysis, results are placed in Appendix D.

# 5. Impact assessment and interpretation

The following chapter covers the last two parts of the life cycle assessment: The impact assessment and the interpretation of results. In this section, the environmental profile of the product systems is presented and discussed, and the product systems are compared. Also included is sensitivity analysis and the uncertainty evaluation.

## 5.1 Base scenario evaluation

The first objective of the study is to compare the potential environmental impact of the three product systems (NaOCl, PAA and PFA) based on the freshwater ecotoxicity and human health impact categories from the USEtox model, and climate change as well as resources from the Impact 2002+ model. Figure 8 and Figure 9 show a comparison of five categories for the product systems for the Venice treatment plant and the NW Langley treatment plant. It is important to keep in mind for the interpretation of results that the context for the two treatment plants is very different: the functional unit, geographic and time scale are different. Furthermore, the limitations of the study and the assumptions made should be taken into consideration.

The graph is presented on a relative scale to avoid comparing the midpoints with each other, as this is not permitted by the ISO 14040 guidelines for an LCA available to the public. Results are calculated relative to the disinfectant with the highest potential impact for each impact category. For example, the total potential impact on freshwater toxicity of NaOCl is $9.03 \times 10^7$ PAF (Potentially affected fraction of species)*$m^2$*d. The total impact of PAA on freshwater toxicity is $1.21 \times 10^7$ PAF*$m^2$*d, 13% of the total potential impact of NaOCl, as seen on Figure 8. Total impacts are presented in Table 10 for the Venice WWTP and in Table 11 for the NW Langley WWTP.

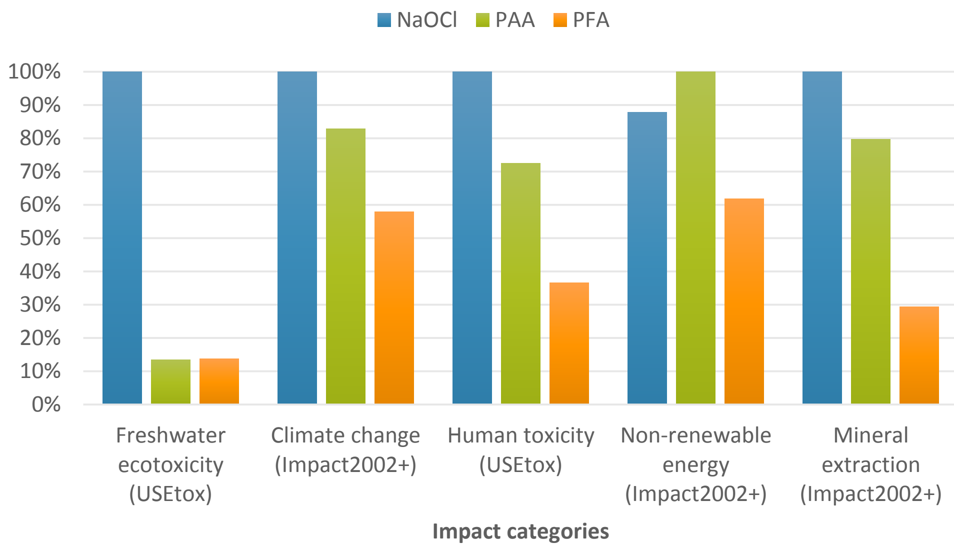



*Figure 8. Impacts of NaOCl, PAA and PFA disinfection on freshwater ecotoxicity, climate change, human health (cancer and non-cancer) and resources (non-renewable energy and mineral extraction) for the* ***Venice WWTP***

*Table 10. Total impacts of NaOCl, PAA and PFA for each midpoint category at the* ***Venice WWTP***

| *Impact category* | *Disinfectant* | *Total impact* | *Units* |
|---|---|---|---|
| | NaOCl | 9.03E+07 | |
| *Freshwater ecotoxicity* | PAA | 1.21E+07 | PAF*$m^2$*d |
| | PFA | 1.25E+07 | |
| | NaOCl | 3.83E+04 | |
| *Climate change* | PAA | 3.17E+04 | Kg eq. $CO_2$ |
| | PFA | 2.22E+04 | |
| | NaOCl | 2.12E-02 | |
| *Human toxicity* | PAA | 1.54E-02 | DALY |
| | PFA | 7.75E-03 | |
| | NaOCl | 6.36E+05 | |
| *Non-renewable energy* | PAA | 7.24E+05 | MJ |
| | PFA | 4.47E+05 | |
| | NaOCl | 2.34E+03 | |
| *Mineral extraction* | PAA | 1.87E+03 | MJ |
| | PFA | 6.87E+02 | |

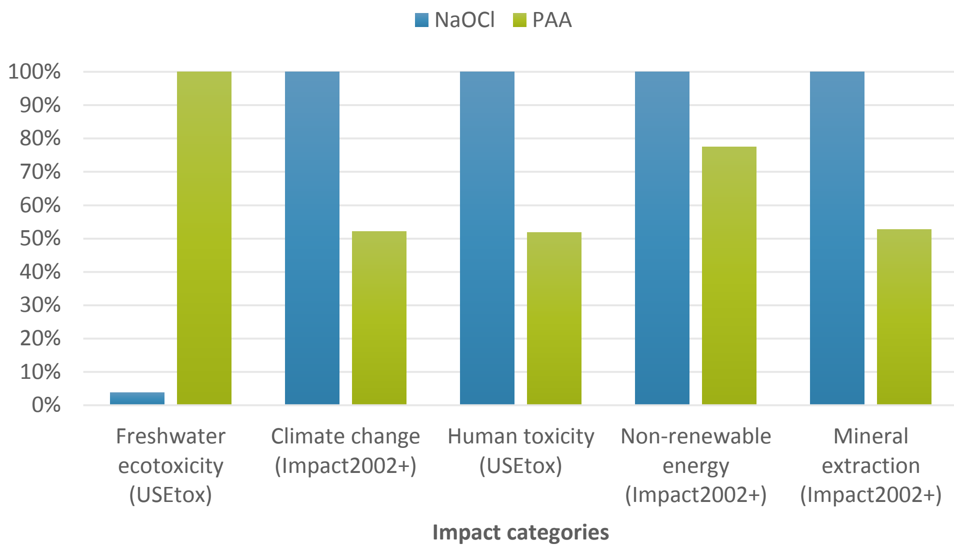



*Figure 9. Impacts of NaOCl and PAA disinfection on freshwater ecotoxicity, climate change, human health (cancer and non-cancer) and resources for the* ***NW Langley WWTP***

*Table 11. Total impacts of NaOCl, PAA and PFA for each midpoint category at the* ***NW Langley WWTP***

| *Impact category* | *Disinfectant* | *Total impact* | *Units* |
|---|---|---|---|
| *Freshwater ecotoxicity* | NaOCl | 9.06E+05 | PAF*m$^2$*d |
| | PAA | 2.36E+07 | |
| *Climate change* | NaOCl | 9.40E+04 | Kg eq. $CO_2$ |
| | PAA | 4.90E+04 | |
| *Human toxicity* | NaOCl | 4.75E-02 | DALY |
| | PAA | 2.46E-02 | |
| *Non-renewable energy* | NaOCl | 1.30E+06 | MJ |
| | PAA | 1.00E+06 | |
| *Mineral extraction* | NaOCl | 5.62E+03 | MJ |
| | PAA | 2.96E+03 | |

### 5.1.1 Freshwater toxicity

#### 5.1.1.1 Venice

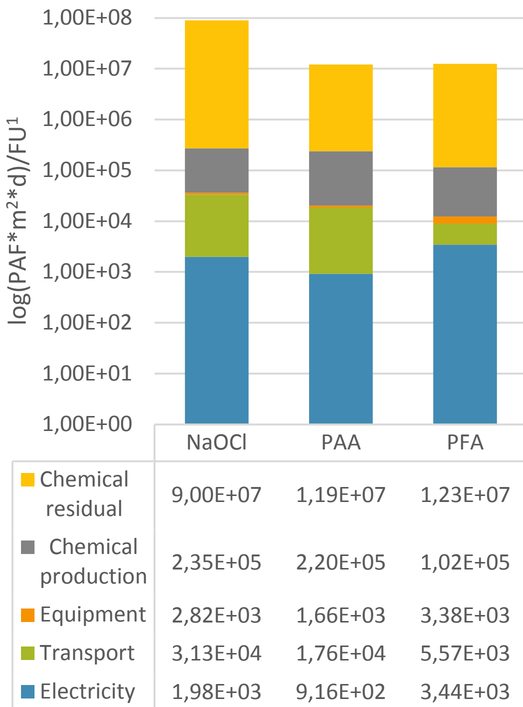
The residuals from disinfection dominate the freshwater impact category. As mentioned before, the USEtox method, at this time, has not developed characterisation factors for four of the residuals from disinfection: performic acid, hydrogen peroxide, sodium bisulfite and free chlorine; therefore, interim characterisation factors were calculated. USEtox has provided the following guidelines in the event that interim CFs are used for an LCA:

- In the absence of recommended characterisation factors, use interim characterisation factors, as excluding interim characterisation factors implies a zero impact hypothesis for the respective emissions. The uncertainty of this hypothesis is usually higher than the uncertainty of the indicative characterisation factors.
- If substances characterised with interim factors dominate impacts of the study, it may be useful to conduct a sensitivity analysis by excluding the interim factors in order to see if the conclusions of the study are affected or not.
- If excluding interim characterisation factors affects the conclusions, it may be justified to leave them out of the study. In that case, one needs to state that the emissions were excluded and in reality may still contribute significantly to the total impacts.

The characterisation factors (potential impact per kg of substance) for freshwater ecotoxicity depends highly on the $EC_{50}$, the concentration that creates an observable effect on half of the aquatic species exposed during tests. $EC_{50}$ values used to determine the interim CFs are shown in Table 2 (Section 2.6). The $EC_{50}$ of PFA being higher than that of PAA, the CF was also higher. However, as Figure 10 demonstrates, the total potential impact of the peracids (PAA and PFA) on freshwater ecotoxicity are very similar. Units for the figures are described in Section 3.2.5. As suggested by Hauschild et al. (2017), the results are shown on a log scale to reflect the uncertainty of the results, and to avoid over-exaggeration of the differences. The oxidation potential of PFA is higher than that of PAA; therefore, the applied dose and residual is smaller for PFA. The reduced residual compensates for the higher characterisation factor of PFA.

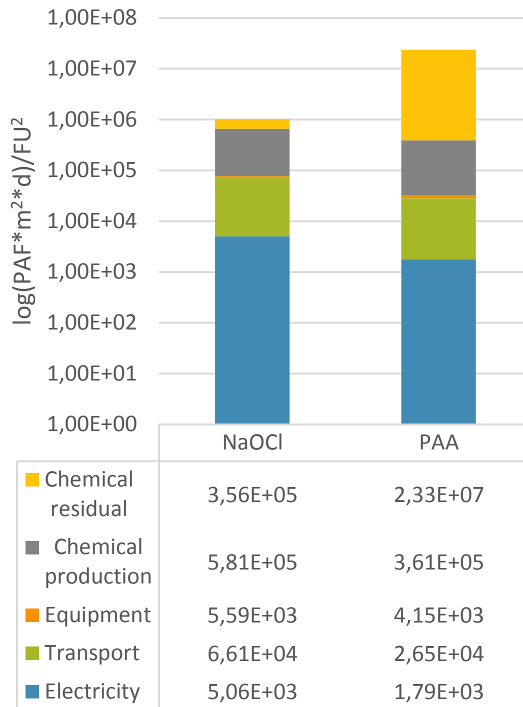
The ecotoxicity of the chlorine residual is one order of magnitude higher than that of the peracids. This is not surprising considering that it is widely recognized that chlorine is toxic to aquatic species at low concentrations (0.04 mg/L). The chlorine residual was divided between free (0.09 mg/L) and combined chlorine (0.62 mg/L).

The potential impacts on freshwater toxicity are clearly dominated by substances characterised with interim factors: free chlorine and performic acid. However, it does not make sense in this case to exclude the interim characterisation factors, as this would entail eliminating the potential impact of residuals for only some disinfectants. Furthermore, the results for freshwater toxicity are compatible with previous research: That chlorine residual is very toxic to aquatic life, and that PFA residual is more toxic than PAA due to its higher oxidation potential. Results indicate that the smaller dose of PFA applied to effluents may compensate for the higher toxicity; however, the interim CFs for chemical residuals need to be externally validated before results are stated with certainty.




| | NaOCl | PAA | PFA |
|---|---|---|---|
| Chemical residual | 9,00E+07 | 1,19E+07 | 1,23E+07 |
| Chemical production | 2,35E+05 | 2,20E+05 | 1,02E+05 |
| Equipment | 2,82E+03 | 1,66E+03 | 3,38E+03 |
| Transport | 3,13E+04 | 1,76E+04 | 5,57E+03 |
| Electricity | 1,98E+03 | 9,16E+02 | 3,44E+03 |

*Figure 10. Comparison of the potential impacts of* ***freshwater ecotoxicity***[1] *of NaOCl, PAA and PFA disinfection at the* ***Venice WWTP***




| | NaOCl | PAA |
|---|---|---|
| Chemical residual | 3,56E+05 | 2,33E+07 |
| Chemical production | 5,81E+05 | 3,61E+05 |
| Equipment | 5,59E+03 | 4,15E+03 |
| Transport | 6,61E+04 | 2,65E+04 |
| Electricity | 5,06E+03 | 1,79E+03 |

*Figure 11. Comparison of the potential impacts of* ***freshwater ecotoxicity***[2] *of NaOCl and PAA disinfection at the* ***NW Langley WWTP***

5.1.1.2 NW Langley

As mentioned, the main difference between the plants used for the study is the additional dechlorination process at NW Langley, as well as the disinfectants used; only NaOCl and PAA were used at NW Langley. For most impact categories, the trends observed (Figure 9) are similar to those observed at the Venice WWTP (Figure 8), with the exception of freshwater toxicity.

[1] Functional unit (FU): 3 log removal of E. *coli* in the effluent over two months at the Venice WWTP.
[2] FU: Effluent disinfection over seven months to a concentration of less than 200 MPN/100 mL fecal coliforms at the edge of the initial dilution zone at the NW Langley WWTP.

Whereas the residual from NaOCl disinfection at the Venice WWTP resulted in the highest potential impact on freshwater toxicity, the added dechlorination with sodium bisulfite at the NW Langley WWTP decreased potential toxicity impacts by a significant amount as shown in Figure 11.

5.1.1.3 Relationship between chemical residual and potential impact

Figure 12 and Figure 13 demonstrate the relationship between residual and potential impact: while the sulfur dioxide residual concentration is very high, the characterisation factor is low which results in a low total potential impact for the residual from NaOCl disinfection at NW Langley. At the Venice WWTP, the residual combined chlorine is comparable in weight to the PAA residual, however the CF for combined chlorine being very high, the total potential impact of the residual is much higher with NaOCl disinfection.

Dechlorination ensured that the free and combined chlorine were removed from the effluent, however, residual sulfate from dechlorination was added in the process. The toxicities of both free chlorine and the sodium bisulfate residual were evaluated using interim characterisation factors.

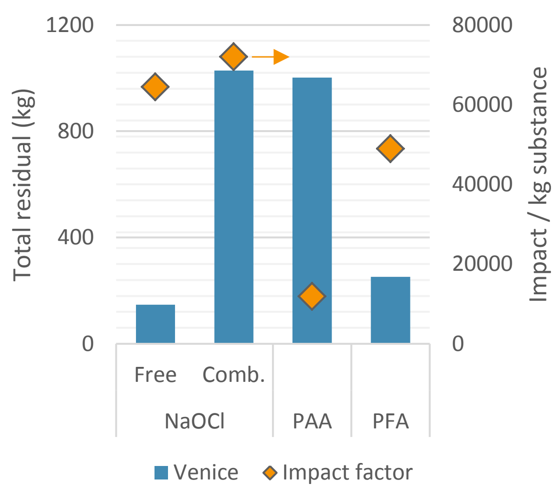



*Figure 12. Impacts on **freshwater toxicity** of NaOCl and PAA residuals at the **Venice WWTP** in relation to the functional unit*

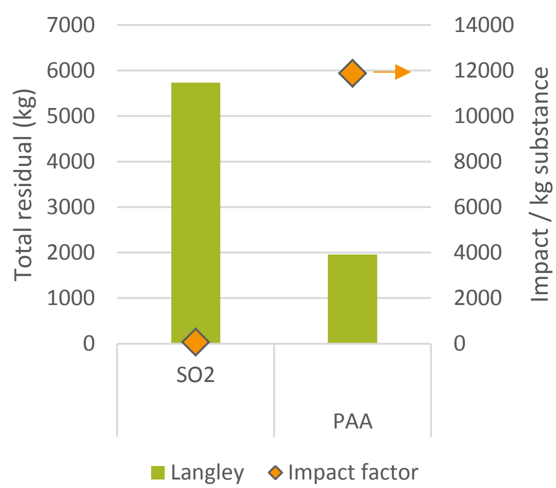



*Figure 13. Impacts on **freshwater toxicity** of NaOCl and PAA residuals at the **NW Langley WWTP** in relation to the functional unit*

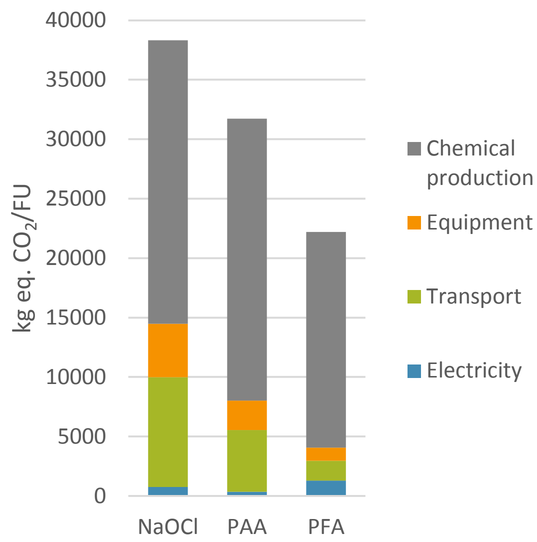
The trends observed with and without dechlorination are different. Dechlorination eliminated the chlorine residual, however, sodium bisulfite was added to the effluent for dechlorination. The CF for sulfate being much smaller than free and combined chlorine (Table 5. ) the total potential impact remained low. At NW Langley, where dechlorination occurred, the potential impact of PAA was one order of magnitude higher than the potential impact of NaOCl disinfection on freshwater toxicity.

### 5.1.2 Climate change

#### 5.1.2.1 Venice

Whereas freshwater toxicity has the highest model uncertainty of all the impact categories, the uncertainty linked to the climate change model is low in comparison (Table 4). The potential impact on climate change of the NaOCl product system, illustrated in Figure 8, is the highest followed by PAA, which has a little over 8% of the total potential impact of NaOCl; PFA has a little more than half the impact of NaOCl. For all product systems, the production of the disinfectant dominate the impacts, as shown in Figure 14. The second most important contributor to potential impacts on climate change is transportation. The hypothetical distance travelled for all components of the LCA is 1000 km; therefore, the difference is due only to the weight of chemicals transportation. For this reason, the potential impact linked to transportation of NaOCl is highest because the dose of NaOCl needed to fulfill the functional unit is higher (Table 8). In contrast, the dose of PFA is the smaller and therefore the potential impact of transportation is smaller.

The production of the disinfectants was broken down further in order to investigate the major contributors, illustrated in Figure 16. As mentioned, the burden of chemical production on climate change is very similar for NaOCl and PAA, whereas it is much less for PFA. Whereas PAA and PFA both require hydrogen peroxide, the production of NaOCl requires chlorine gas and sodium hydroxide. A comparison of the production of NaOCl, PAA and PFA based on weight produced instead of dose is included in section 5.1.6. More hydrogen peroxide is necessary for PAA production, in relationship to the dose. The potential impact of the chemical factory construction is also higher for NaOCl due to the higher dose: a larger fraction of chemical factory is needed. As PFA is produced on-site, the chemical factory construction potential impact is not presented on the figures. PFA does however require a cooling unit, which is included in the equipment and the electricity. Production of NaOCl requires steam; the heat contributes to over 20% of the total potential impacts of NaOCl production.



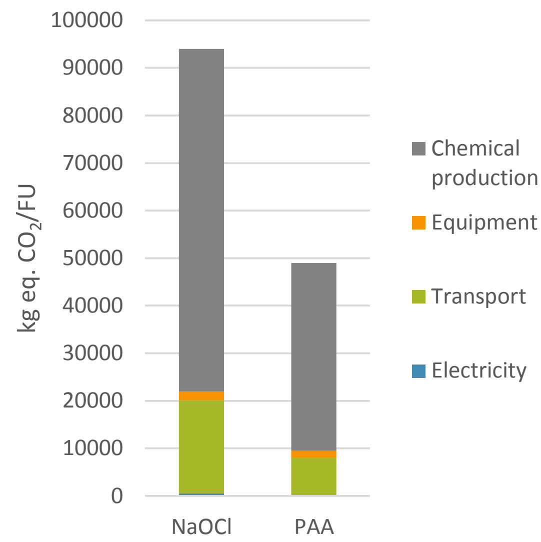
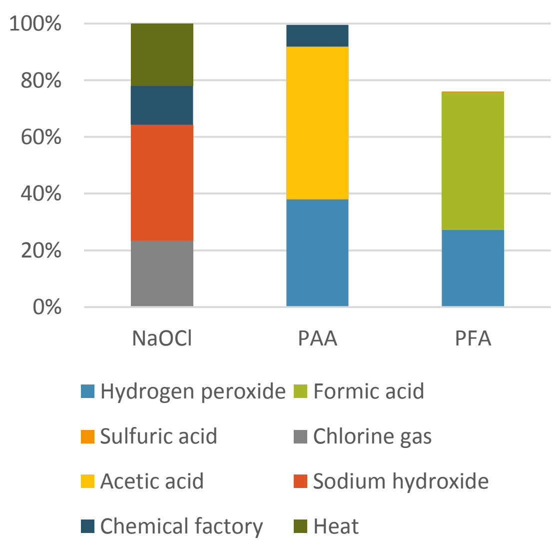




*Figure 14. Comparison of the impacts of **climate change** of NaOCl and PAA disinfection at the **Venice WWTP***

*Figure 15. Comparison of the impacts of **climate change** of NaOCl and PAA disinfection at the **NW Langley WWTP***



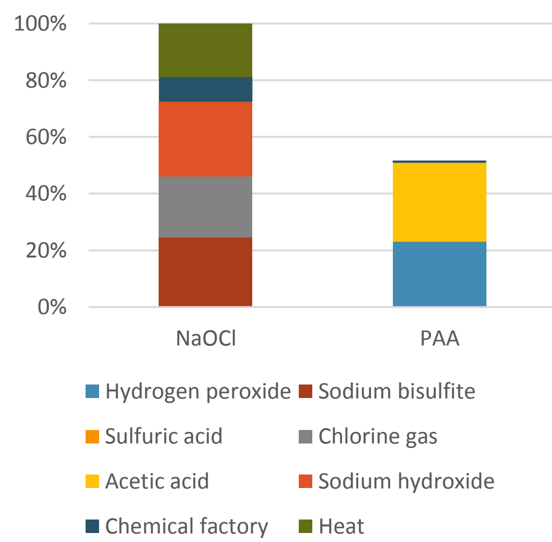




*Figure 16. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **climate change** at the **Venice WWTP***

*Figure 17. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **climate change** at the **NW Langley WWTP***

#### 5.1.2.2 NW Langley

The potential impact on climate change of NaOCl disinfection at the NW Langley treatment plant is also higher than for PAA disinfection. The difference in potential impacts between NaOCl and PAA is however less pronounced than at the Venice WWTP. Whereas the potential impact of PAA disinfection at NW Langley is nearly 50% smaller than impact of NaOCl disinfection, it is little over 15% smaller at the Venice treatment plant. This is due to the added dechlorination process, which contributed significantly through added chemical production, described in Figure 17. At NW Langley, the production of sodium bisulfite contributes to 25% of total potential impacts due to chemical production, on climate change. As for transportation, the impacts follow the same trend as for the Venice treatment plant.

### 5.1.3 Human Toxicity

#### 5.1.3.1 Venice

From Figure 8, the potential impacts on human toxicity of the three product systems follow the same trend as for climate change: The toxicity of NaOCl is the highest, followed by PAA and then PFA. The potential human toxicity impacts do not include the residuals in the treatment plant effluent, as the characterisation factors for the potential impact on human health could not be developed due to limited knowledge about their fate in the environment, the exposure, and the effect of the residuals on human toxicity. Once again, total potential impacts are dominated by chemical production, shown in Figure 18. Transport is the second most important contributor to human toxicity, and the relationship follows a trend proportional to the dose of disinfectant. In terms of chemical production, from Figure 20, 50% of the impacts of NaOCl production are from chemical factory construction (emissions of zinc and arsenic to water are largely responsible); sodium hydroxide and chlorine gas each account for half of the remaining total potential impact. The potential total impact of PAA production is about 75% of the total impacts of NaOCl, and PFA is less than 40%. For both PAA and PFA production, the potential impacts of hydrogen peroxide are very important. The only chemical residual for which a human toxicity characterisation factor has been developed is chloramines (seen in Figure 18), but it is small. The potential impacts on human toxicity of PAA and PFA residuals are still unknown and are not shown.

5.1.3.2 NW Langley

The potential impact on human toxicity at the NW Langley follows the same trend set by the Venice treatment plant. The total potential impact of PAA disinfection is approximately half that of NaOCl disinfection. Potential impacts are dominated by chemical production once again. From Figure 21, the potential impacts of chemical production are due to the chemical factory construction, and the production of hydrogen peroxide, acetic acid, sodium hydroxide, sodium bisulfite, heat, and chlorine gas.

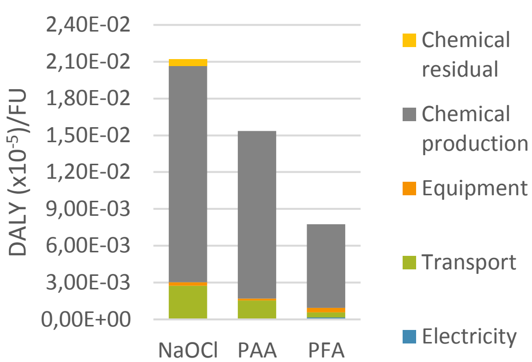



*Figure 18. Comparison of the impacts on **human toxicity** of NaOCl and PAA disinfection at the **Venice WWTP***

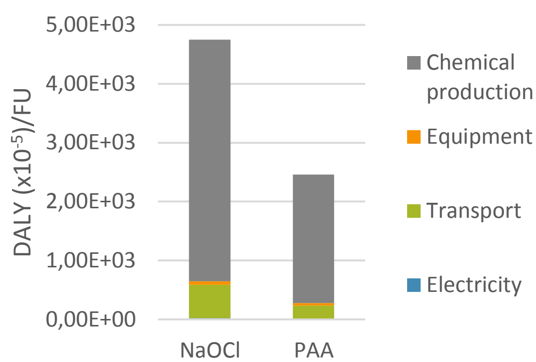



*Figure 19. Comparison of the impacts on **human toxicity** of NaOCl and PAA disinfection at the **NW Langley WWTP***

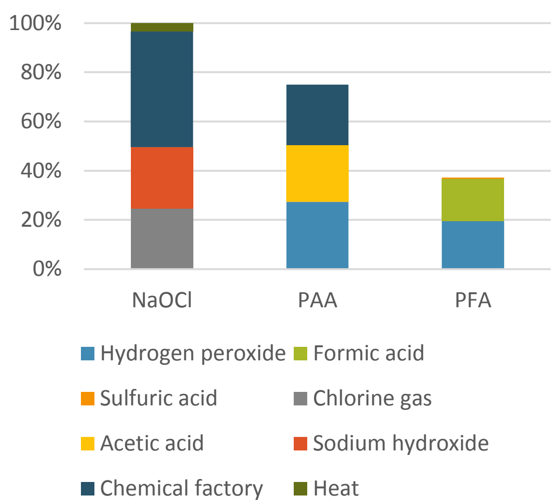



*Figure 20. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **human toxicity** at the **Venice WWTP***

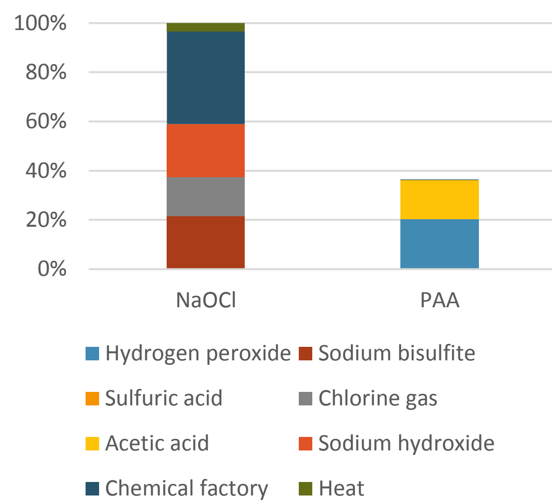



*Figure 21. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **human toxicity** at the **NW Langley WWTP***

### 5.1.4 Non-renewable energy

#### 5.1.4.1 Venice

The use of non-renewable energy is the only impact category for which the potential impact of PAA is the highest. The main contributor to total potential impacts for all disinfectants is chemical production: for PAA, chemical production accounts for nearly 77% of total potential impacts on non-renewable energy (Figure 22). From Figure 23, PFA disinfection has the lowest potential impact on non-renewable energy, with little less than 60% of the potential impacts of PAA disinfection. The potential impacts of production of PAA are mainly due to the production of acetic acid, followed by hydrogen peroxide, seen in Figure 24. For PFA production, formic acid contributes the most, followed by hydrogen peroxide as well. NaOCl has the smallest potential impact, comprising chemical factory construction, sodium hydroxide, heat and chlorine gas.

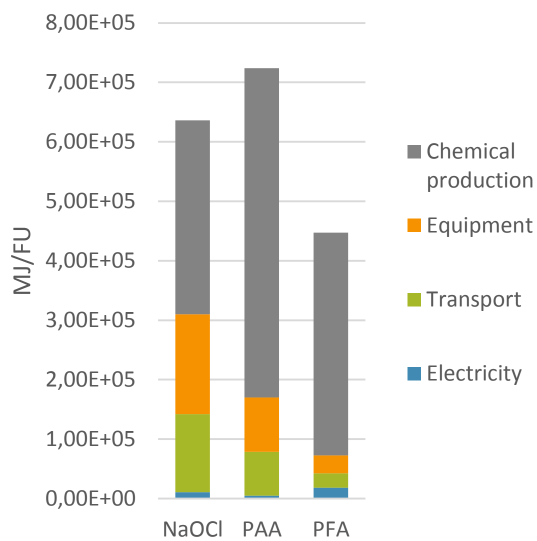



*Figure 22. Comparison of the impacts on **non-renewable energy** of NaOCl and PAA disinfection at the **Venice WWTP***

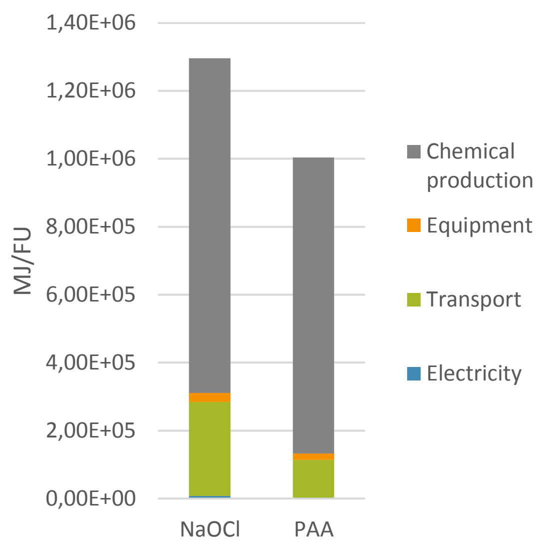



*Figure 23. Comparison of the impacts on **non-renewable energy** of NaOCl and PAA disinfection at the **NW Langley WWTP***

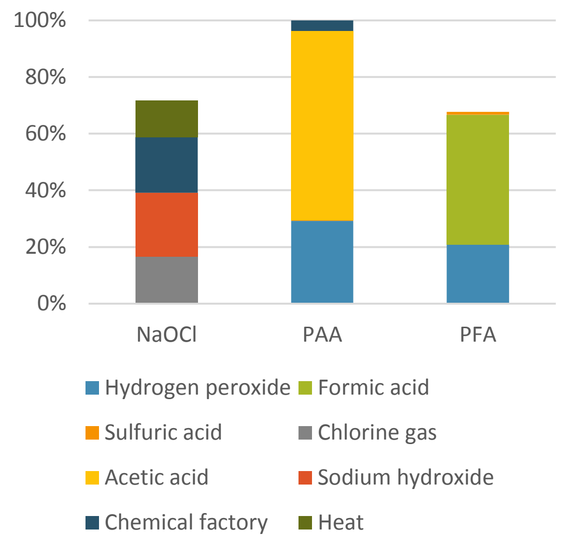



*Figure 24. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **non-renewable energy** at the **Venice WWTP***

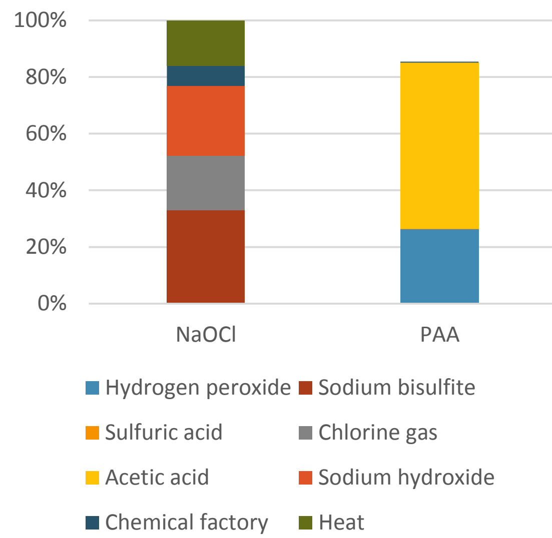



*Figure 25. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **non-renewable energy** at the **NW Langley WWTP***

#### 5.1.4.2 NW Langley

The added dechlorination step at the NW Langley treatment plant reverses trends observed for the Venice WWTP (NaOCl vs PAA only). At NW Langley, the potential impact of NaOCl disinfection is higher than for PAA, shown in Figure 23, due to the important contribution of sodium bisulfate production (33%) to the production of chemicals, which is the most important contributor to non-renewable energy consumption (Figure 25).

### 5.1.5 Mineral Extraction

#### 5.1.5.1 Venice

The potential impact of total mineral extraction of the three disinfectants follows the trend set by the dose: The potential impact of NaOCl is the highest, followed by PAA and PFA. While the potential impact of PAA is over 20% less than that for NaOCl, for PFA it is 75% less (Figure 8). From Figure 28, chemical production dominates potential impacts for all product systems; NaOCl production is dominated by the chemical factory construction (73% of total impacts); the remaining potential impacts are shared in equal proportion by production of sodium hydroxide production and chlorine gas. The potential impact of construction of the chemical factory is mainly due to the use of nickel and copper. The proportion of potential impacts due to the production of chemicals is smaller for PAA, because of the lower dose. Acetic acid and hydrogen peroxide production have an almost equal share of the total potential impacts.

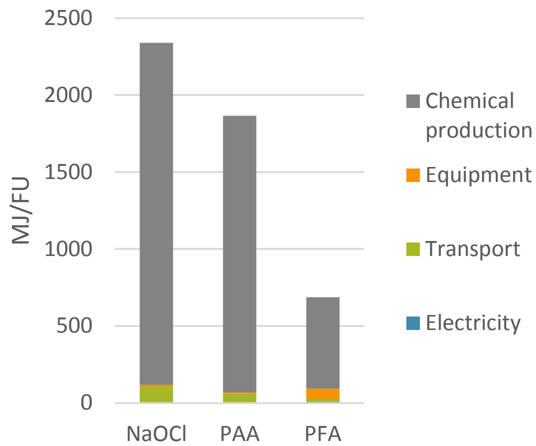



*Figure 26. Comparison of the impacts on **mineral extraction** of NaOCl and PAA disinfection at the **Venice WWTP***

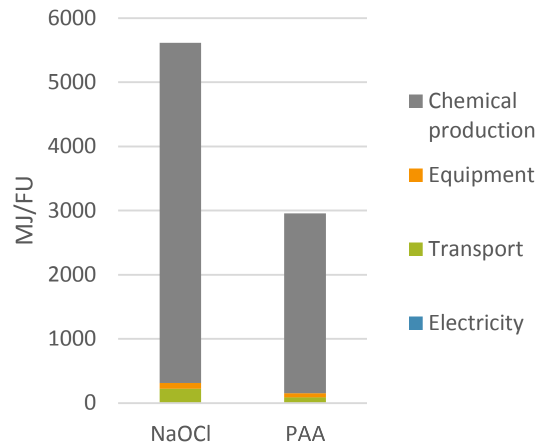



*Figure 27. Comparison of the impacts on **mineral extraction** of NaOCl and PAA disinfection at the **NW Langley WWTP***

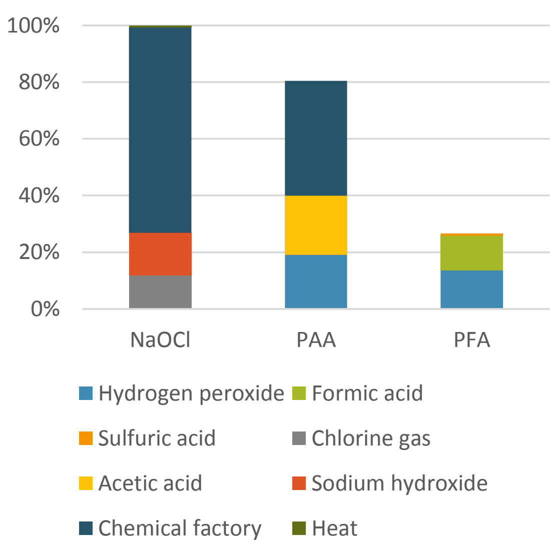



*Figure 28. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **mineral extraction** at the **Venice WWTP***

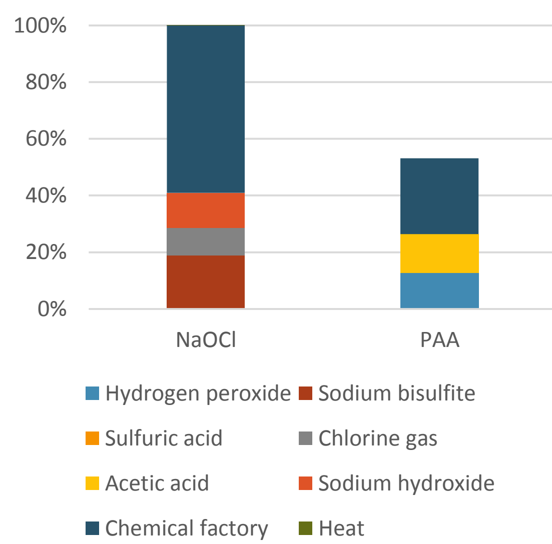



*Figure 29. Comparative contribution of the inputs for **disinfectant production** to the total impacts of chemical production on **mineral extraction** at the **NW Langley WWTP***

5.1.5.2 NW Langley

The most important contributor to potential impacts on mineral extraction is the production of chemicals, therefore the same trend is observed as previously: The difference between the two disinfectants is higher due to the additional process of sodium bisulfate production (Figure 29), and PAA has about 50% less impact that NaOCl.

### 5.1.6 Impacts of chemical production

As mentioned above, the potential impacts attributed to chemical production are based on the functional units for each treatment plant, and therefore the doses of each disinfectant are different. The potential impacts of NaOCl production, for example, are very high due to the comparatively high dose of NaOCl needed for adequate disinfection. It is therefore interesting to compare all three disinfectants **based on the production of 1 kg** so that the impacts are not influenced by the required dose at the treatment plants. The comparison is shown in Figure 30.

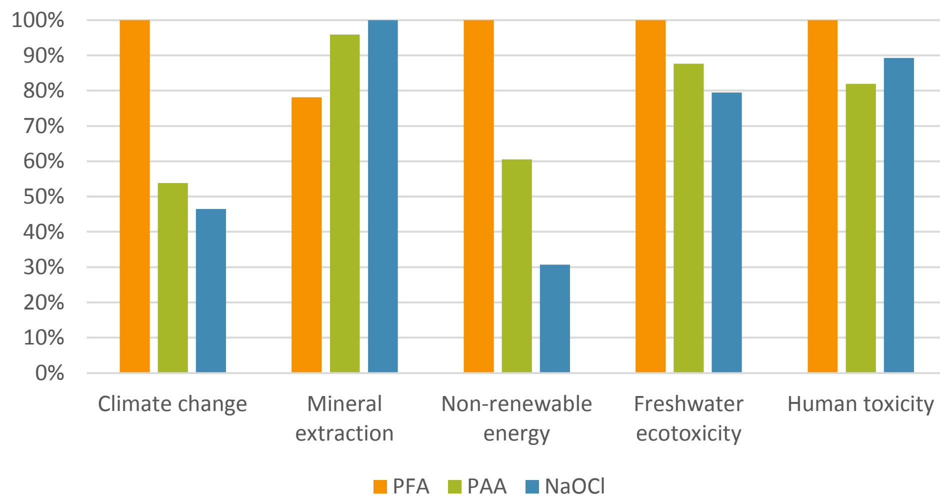



*Figure 30. Impacts of NaOCl, PAA and PFA based on the production of 1 kg*

Figure 30 shows a different trend from that in previous sections. Whereas the potential impacts of PFA production were always lowest when chemical production was calculated as a function of the functional unit, here the potential impacts of production are the highest for PFA, for all impact categories with the exception of mineral extraction. The full breakdown of the potential impacts of chemical production is included in Appendix F.

The two most important contributors to the potential impact of PFA production are hydrogen peroxide and formic acid production. While PAA also requires hydrogen peroxide, the quantity is smaller per kg produced. The impact of formic acid is especially high because it requires carbon monoxide, which in turns requires a large amount of electricity and some heavy fuel oil. Acetic acid, the main contributor to potential impacts of PAA production, also requires carbon monoxide for production, but in much smaller quantity. The principal contributor to potential impacts of NaOCl production are sodium hydroxide production, chlorine gas production and heat used to produce steam.

From Figure 30, it can be concluded that while impacts of PFA per kg of active substance produced are higher than PAA and NaOCl, the low dose of PFA needed for adequate disinfection compensates for the high impact of production. Furthermore, the smaller amount of disinfectant produced also reduces transportation impacts.

## 5.2 Uncertainty analysis

The uncertainty analysis has two main objectives: First, to evaluate the uncertainty of the input data, and second, to evaluate how the data uncertainty influences the LCA results.

There are three types of uncertainty in LCA: Parameter uncertainty, scenario uncertainty as well as model uncertainty. Parameter uncertainty is expressed as a distribution of the possible values of a parameter, using a probability distribution function. It is difficult to obtain a sufficient amount of data to parameterize a lognormal or Gaussian distribution (the most frequently used distribution for parameter uncertainty), therefore uncertainties are often evaluated using qualitative indicators (Jolliet et al., 2016).

Model uncertainty comes from the simplifications of reality made in order to model processes occurring in the environment. For example, effects are often considered linear when this is not always the case. Furthermore, the models often contain extrapolations, such as the use of the octanol-water partition coefficient to evaluate bioconcentration factors for chemicals.

Uncertainty also comes from choices and assumptions made by the LCA practitioner in the definition of the goal and scope. In some LCAs, the functional unit or the choice of system boundaries can influence the results of the study. Finally, uncertainty is also contributed by factors such as spatial and temporal scales. Most LCAs contains global supply chains, which makes it difficult to calculate impacts in small spatial scales, and they contain technologies for which performance varies over time.

Humbert, Rossi, Margni, Jolliet & Loerincik (2009) have defined the following “rules of thumb” for uncertainty in LCA: 10% for climate change and resource consumption, and one order of magnitude for environmental and human toxicity. However, these rules, being based on experience, and not on an objective analysis, are not sufficient to provide any real analysis on the uncertainty of a study. For this reason, the uncertainty is evaluated for this study using the method described below.

For most of the data that it contains, the ecoinvent database uses the lognormal distribution for two reasons: First, the lognormal distribution is frequently observed in real life populations due to their multiplicative rather than additive effects. Second, most parameters for real life populations are always positive, and the standard deviation of the underlying normal distribution is scale independent. Furthermore, two types of uncertainty are quantified in ecoinvent:

1. Basic uncertainty: Variation and stochastic error of the values that describe the exchanges (measurements, activity specific variations, temporal variations).
2. Additional uncertainty via quality indicators: Due to estimates, lack of verification, incompleteness, extrapolation, the use of temporally or geographically different conditions.

The additional uncertainty is added using the pedigree approach. The pedigree matrix used for uncertainty analysis and the associated default uncertainty factors are given in Appendix H. A Monte Carlo simulation is then used in order to propagate the two types of uncertainties.

The uncertainty assessment described above does not include model uncertainty as well as mistakes imposed by human error. In order to evaluate whether model uncertainty can affect the results of the study, sensitivity analysis is performed in Section 5.3.

To calculate the parameter uncertainty, the product systems were subtracted from each other in order to determine the uncertainty of the difference between the impact scores, and a Monte Carlo simulation was performed on the result. This subtraction was done because the focus of the study is not how large the impact of the product systems is, but rather how large is the <u>difference</u> between the impacts of the product systems. Furthermore, this method removes uncertainty of correlated parameters (parameters that are present in both product systems such as transport) which avoids overestimating the uncertainty. This is done for both models used, Impact 2002+ and USEtox. The uncertainty range, the range of values where a certain proportion of all randomly measured values can be found, is 95% (Hauschild et al., 2017). It was determined that 1 000 iterations would be sufficient, as the uncertainty measures such as mean and standard deviation did not change significantly with additional iterations. It is important to note that parameter uncertainty is calculated not because it is the most important type of uncertainty, but because it is the more accessible one.

### 5.2.1 Venice WWTP

The results presented in Section 5.1 for the Venice WWTP indicate that the potential impact on freshwater ecotoxicity of NaOCl is the highest, and that the impacts of PFA are slightly above those of PAA. The Monte Carlo analysis, which is developed in full in Appendix I, indicates low parameter uncertainty of freshwater toxicity. Considering that the total impact is more than 98% due to the residual, this is not surprising as impacts are generally due to one parameter. Considering that interim factors were used, the model uncertainty for freshwater toxicity is very high; however, the model uncertainty cannot be quantified in the same way as parameter uncertainty, which was quantified using the Monte Carlo method.

According to the results of the Monte Carlo analysis, illustrated in Table 12, NaOCl as a higher potential impact than PAA in all the simulations, and PAA has a higher impact than PFA in all impact categories except ecotoxicity.

*Table 12. Calculated probabilities for the LCA results using Monte Carlo simulations for the Venice WWTP*

| | *Ecotoxicity* | *Climate change* | *Human toxicity* | *Non-renewable energy* | *Mineral extraction* |
|---|---|---|---|---|---|
| *NaOCl > PAA* | 100% | 77% | 68% | 100% | 67% |
| *PAA > PFA* | 25% | 100% | 100% | 100% | 100% |

### 5.2.2 NW Langley WWTP

Results from the Monte Carlo simulations for the NW Langley WWTP, in Table 13, indicate that there is little overlap between the two product systems: The impact of NaOCl disinfection is higher in 100% of scenarios for climate change and human toxicity. For non-renewable energy use and mineral extraction, the likelihood of NaOCl having a higher potential impact is respectively 98% and 97%. Impacts of PAA on freshwater toxicity are higher than NaOCl in 100% of the simulations. As mentioned, the model uncertainty for freshwater toxicity is not accounted for in these results.

*Table 13. Calculated probabilities for the LCA results using Monte Carlo simulations for the NW Langley WWTP*

| | *Ecotoxicity* | *Climate change* | *Human toxicity* | *Non-renewable energy* | *Mineral extraction* |
|---|---|---|---|---|---|
| *NaOCl > PAA* | 0% | 100% | 100% | 98% | 97% |

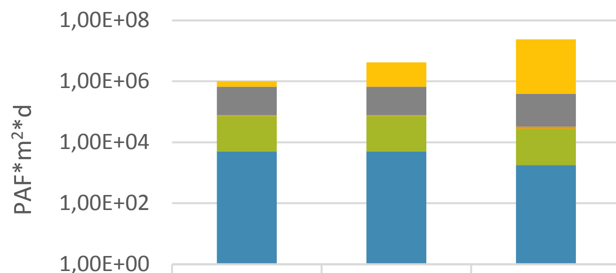
## 5.3 Sensitivity analysis

As mentioned, the uncertainty analysis performed above could not take into account model uncertainty. Therefore, sensitivity analysis was used to determine whether the conclusions of the study could be significantly impacted by model uncertainty. The model uncertainty is due to the calculation of the characterisation factors, which indicate the impact per kg of substance released into the environment.

### 5.3.1 Characterisation factors

#### 5.3.1.1 Sulfate

The residual from sodium bisulfate dechlorination being sulfate, an ionic and non-organic chemical species, the USEtox model only provides an approximation for the characterisation factor. For this reason, impacts are calculated by varying the characterisation factor obtained with the model in order to determine how results are affected. From Table 5 (Section 3.2.5), the characterisation factor calculated for sulfate is 62 PAF*$m^2$*d/kg. For the sensitivity analysis, the CF for sulfate is increased by one order of magnitude to 620 PAF*$m^2$*d/kg. Results are shown in Figure 31.




| | NaOCl (CF=62) | NaOCl (CF=620) | PAA |
|---|---|---|---|
| Chemical residual | 3,56E+05 | 3,55E+06 | 2,33E+07 |
| Chemical production | 5,81E+05 | 5,81E+05 | 3,61E+05 |
| Equipment | 5,59E+03 | 5,59E+03 | 4,15E+03 |
| Transport | 6,61E+04 | 6,61E+04 | 2,65E+04 |
| Electricity | 5,06E+03 | 5,06E+03 | 1,79E+03 |

*Figure 31. Comparison of the potential impacts of freshwater ecotoxicity of NaOCl and PAA disinfection at the Northwest Langley WWTP with characterisation factors for sulfate of 62 and 620 PAF*m$^2$*d/kg*

Increasing the CF for sulfate results in an increase of the potential impact on freshwater toxicity of one order of magnitude. The total potential impact remains lower than for disinfection with PAA. The characterisation factor could be increased by another order of magnitude, and this would make the impact of NaOCl disinfection similar to the impact of PAA. However, the uncertainty linked to toxicity is usually within one order of magnitude (Humbert et al., 2009).

5.3.1.2 Free chlorine

The characterisation factor (CF) for free chlorine, being non-organic, is only an approximation of the toxicity of the substance to aquatic species. Research has indicate that the toxicity of free and combined chlorine is of the same order of magnitude (Brungs, 1973), therefore, the CFs should be similar. The CF obtained for combined chlorine is classified as “recommended” as it has been validated externally, which is not the case for free chlorine. Furthermore, the calculated CF for free chlorine is one order of magnitude higher than the CF of combined chlorine. Sensitivity analysis is used to investigate whether lowering the potential impact of free chlorine to the same order of magnitude as combined chlorine significantly affects results, shown in Figure 32.

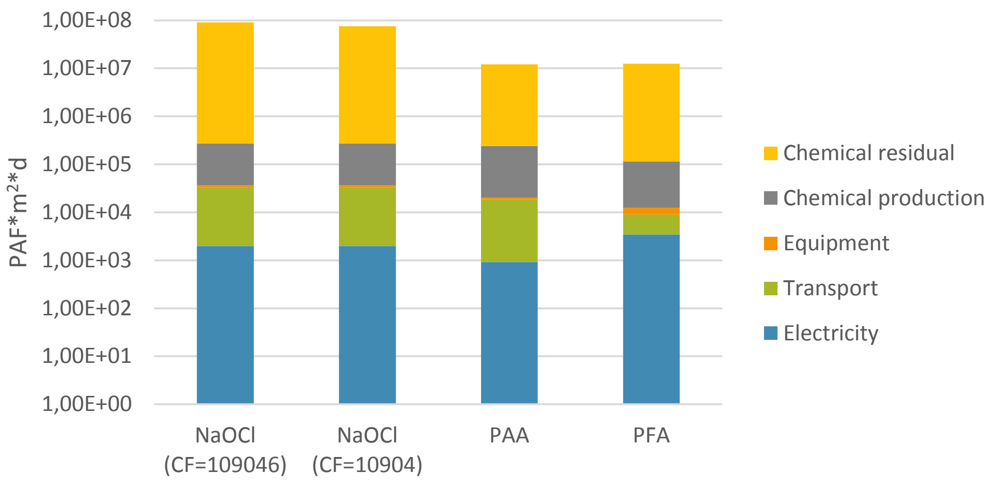



*Figure 32. Comparison of the potential impacts of freshwater ecotoxicity of NaOCl, PAA and PFA disinfection at the Northwest Langley WWTP with characterisation factors for free chlorine of 109 046 and 10 904 PAF*m$^2$*d/kg*

The figure above demonstrates that lowering the CF for free chlorine by one order of magnitude does not change the general trends observed in results. This can be explained by the fact that the residual contains a high amount of combined chlorine and little free chlorine in comparison.

At the Langley treatment plant, the free chlorine residual was determined to be zero by daily testing of the effluent, therefore the results would not be affected. Because the focus of the study is not the total impact of each product system, but the difference between their total impacts, in this case sensitivity analysis does not affect the results of the study.

5.3.1.3 Performic acid and peracetic acid

The results obtained by examining the Venice treatment plant indicate that the toxicity of the peracids is very similar when compared to NaOCl residuals. From the parameter uncertainty analysis, it was found that there is a 75% chance that the total impact of PFA on ecotoxicity is higher than PAA. The CF for PFA is much higher than for PAA; however, the residual for PFA is much smaller, which results in similar total potential impacts on aquatic toxicity. The residuals from disinfection being responsible for over 98% of the total potential impacts on freshwater toxicity for PAA and PFA, increasing or decreasing the CF for either product system would significantly affect the total potential impacts. Increasing the CF for PAA would result in higher potential impacts for PAA than for PFA and vice versa. Therefore, before any results can be stated with certainty, the characterisation factors for PAA and PFA need to be validated externally.

### 5.3.2 Contact tank and disinfection equipment

Due to high uncertainty linked to the amount of concrete in the contact tank, the amount of concrete needed for construction at the Venice treatment plant was doubled in order to observe how impacts would be affected. Results, given in Appendix G, show a minor increase in impacts (less than 6% for all impact categories over the entire life cycle), indicating that the amount of concrete used in these product systems is of minor importance compared to other components of the LCA. The same reasoning could be applied to the equipment used for disinfection. Due to the lack of precise information from the treatment plants, the uncertainty of the impacts are high, however, the total impact of equipment being quite low for all impact categories compared to other LCA components such as chemical production, variations in quantities would not significantly change the conclusions of the study.

## 5.4 Limits of the LCA

LCA is a relatively new science, and more work needs to be done in order to reduce model uncertainty. Both the USEtox and the Impact 2002+ are leading models in the field; however, they still contain many limitations.

For USEtox, the first limitation comes from the approach used for the model, which is appropriate for non-ionic, organic chemicals in a liquid or gaseous state.  Adjustments can be made for inorganic species, metals and partially or fully ionized organic species; however, the calculations are not as reliable. The interim characterisation factors developed for the study were for inorganics; therefore, the uncertainty of the calculation is higher. Additionally, the human toxicity impacts did not consider the possible toxicity of the chemical residuals. This was due to the absence of recommended CFs and the impossibility to calculate interim CFs as too little is known about the residuals' fate, exposure and response.

Furthermore, the models contain inherent limitations due to the spatial and time scales. USEtox is a lumped systems coarse-dimension-scale model (Usetox®, 2017), which means it uses compartments to represent components of the environment. The model takes into account variations between urban, regional and global environments, but considers the compartments as uniform, which is a simplification of reality. All emissions occurring over time and space are aggregated into one flux into the environment; therefore, the results do not constitute a risk assessment, as the specific exposure to substances is not known. As for the time scale, the USEtox model is designed to consider long-term effects, however the model considers the concentrations constant over the exposure duration.

The limitation from the Impact 2002+ model comes from the time scale used for short and long-term emissions. Long-term emissions are considered to occur after 100 years. Short and long-term emissions are considered as equally harmful; however, their occurrence at different times makes this difficult to validate. Furthermore, the model does not account for the impacts of one impact category on another. For example, in theory climate change could affect water quality, which in turn could increase potential impacts on ecotoxicity. The models are, at this time, unable to calculate such impacts.

The study is also limited by the quality and the quantity of data available. For example, data from the ecoinvent database is theoretical in many cases, and is therefore not a completely accurate representation of reality. Furthermore, it was impossible to obtain data from the same types of sources (treatment plants, manufacturers or theoretical calculations for example) for all three disinfectants: the information on the production of PFA is from the Venice treatment plant and is field data, whereas the information for the production of NaOCl was calculated theoretically.

Some processes could not be included in the LCA due to lack of quality data. This was the case for pumps, since some disinfectants such as NaOCl require pumps made with specific materials, but the exact materials of the pumps could not be determined, therefore the same pump was used for all product systems.

Finally, as mentioned, the LCA does not account for disinfection by-products such as THMs from NaOCl disinfection. THMs are a higher concern for drinking water treatment plants than for wastewater treatment plants; nevertheless, it could be useful for future LCAs to include an analysis of THMs. The USEtox database does include characterisation factors for many THMs, described in Table 14. If information on residuals cannot be provided, an analysis based on theoretical calculations could be included.

*Table 14. USEtox characterisation factors for THMs*

| *THM* | *Ecotoxicity CF* | *Human toxicity CF* |
|---|---|---|
| *Dibromochloromethane* | 108.44 | 6.85E-07 |
| *Trichloromethane* | 41.15 | 1.35E-06 |
| *Tribromomethane* | 189.47 | 4.03E-07 |
| *Bromodichloromethane* | 21.47 | 2.82E-06 |
| *Chlorodifluoromethane* | n/a | 6.72E-09 |
| *Chlorofluoromethane* | n/a | 1.61E-06 |
| *Trichlorofluoromethane* | n/a | 4.61E-08 |
| *Dichloromethane* | 14.60 | 6.42E-07 |
| *Bromochloromethane* | 64.94 | n/a |

*Source: usetox.org, 2017*

# 6. Conclusions

The goal of the study was to determine which of the three wastewater disinfectants − sodium hypochlorite, peracetic acid and performic acid, has the lowest potential impact on the environment when considering freshwater toxicity, climate change, human toxicity and resource depletion. This was done with the objective of helping decision makers choose the most environmentally friendly disinfectant for new or upgraded treatment plants. For the analysis, data from two treatment plants were used: A treatment plant in the Venice area of Italy, which has used NaOCl, PAA and PFA for disinfection, and the Northwest Langley treatment plant near Vancouver, Canada, which used NaOCl in the past, with dechlorination, and now uses PAA for disinfection.

The functional unit at the Venice WWTP was the removal of 3 log of *E. coli* at a flow of 27 MLD during the months of August and September. At the NW Langley WWTP, the functional unit was the disinfection of the effluent to less than 200 MPN/100 mL at a flow of 11.5 MLD during the months of April to October.

Results from the Venice WWTP indicate that NaOCl disinfection without dechlorination has the highest potential impact for all categories except for mineral extraction. PFA has the lowest potential impact for all impact categories except for freshwater toxicity, where the impact of PFA is slightly higher than PAA. Uncertainty analysis indicates there is a 75% probability that the impact of PFA is higher than PAA for ecotoxicity. Results from the NW Langley WWTP indicate that dechlorination significantly reduces the impact on ecotoxicity of NaOCl disinfection, compared to PAA. However, the potential impact of climate change, human toxicity and resource depletion increases due to the added environmental burden of the dechlorination process.

The results obtained using the USEtox model for freshwater toxicity depend heavily on interim characterisation factors. In order to reduce the uncertainty of the study, it would be pertinent to conduct further research on the impacts that performic acid, hydrogen peroxide, sodium bisulfite and free chlorine have on freshwater toxicity, and use the newfound information to develop recommended characterisation factors that are more reliable. Another way to lower uncertainty would be to improve the method used to calculate interim characterisation factors, as the present method used is appropriate for non-ionic organic substances. A method better adapted to inorganic ionic substances would lower the uncertainty of the results. As mentioned, the potential impacts of chemical residuals on human health could not be included in the study due to the lack of research on the effects of these chemicals. Therefore, more research in this area would be valuable.

As expected, the results for both treatment plants indicate a relationship between the dose of disinfectant used and the total potential impacts. Based on the production of 1 kg of active substance, the impact of PFA production is the highest, however the applied dose of PFA at the treatment plant being significantly smaller than NaOCl and somewhat smaller than PAA, the impacts are lower for most impact categories when considering the functional units for both treatment plants. For climate change, human toxicity and resource depletion, the production of the chemicals is the most important contributor to total impacts. For ecotoxicity, the chemical residuals contribute to over 98% of total impacts in most cases.

The choice of which disinfectant to use depends on the environmental concerns of the decision makers. In order to choose, a decision matrix or weighting factors could be used. The choice of disinfectant also depends on government regulations. For example, the NW Langley treatment plant was motivated to change from NaOCl to PAA disinfection due to the change in Canadian regulations on the chlorine content of treatment plant effluents, which made compliance much more difficult. The choice of chemical disinfectant also depends on cost and technologies available. The DesinFix unit is only being used in Europe; at this time the US EPA and the Canadian government have not yet approved the use of PFA for wastewater disinfection.

Nonetheless, with upcoming reviews in regulations, PFA could soon be available in more countries. As mentioned, the cost per kg of PAA is higher than for NaOCl. The dose of PAA is however smaller, hence a cost analysis would give more information on the economic benefits of using one disinfectant over another.

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## Appendix A. Sources of electricity in Italy and British Columbia, Canada

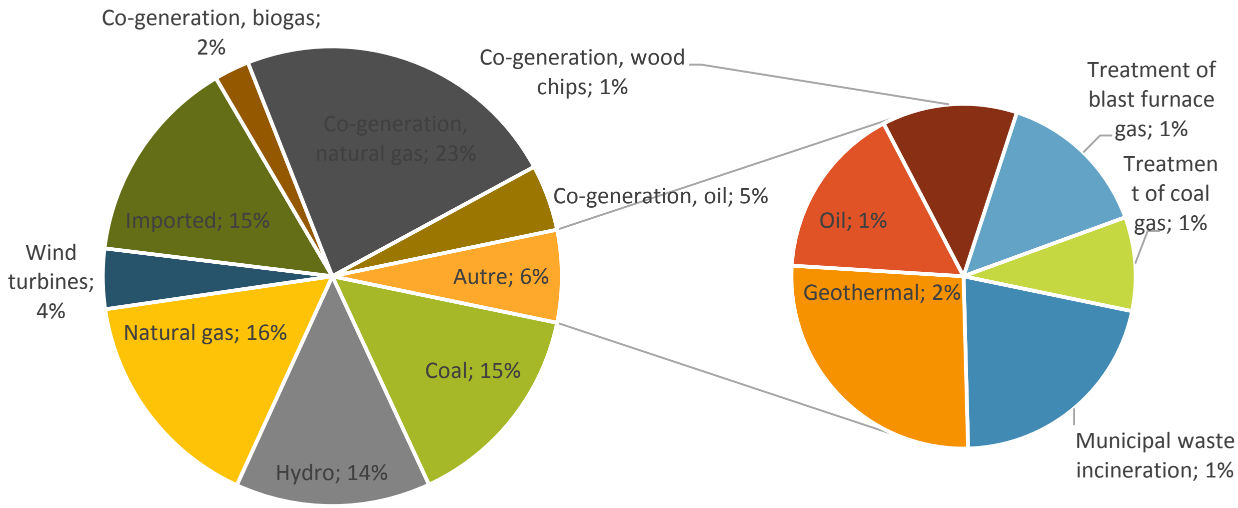



*Figure A 1. Sources of electricity in Italy*
*Source: Wernet et al., 2016*

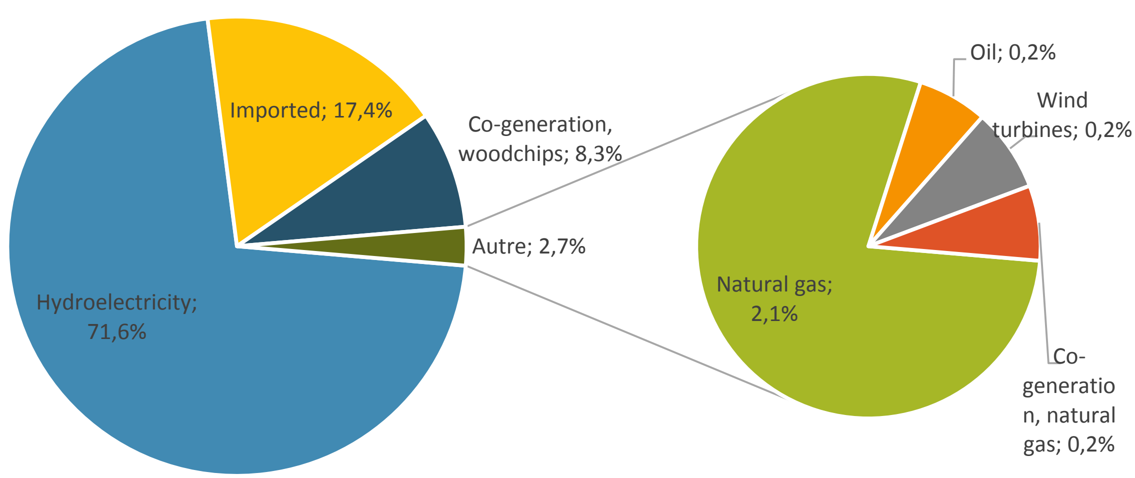



*Figure A 2. Sources of electricity in British Columbia, Canada*
*Source: Wernet et al., 2016*

## Appendix B. Calculations for PAA dose and residual at the Venice WWTPP

To determine the dose of PAA needed at the Venice WWTP to obtain 3 log removal of *E. coli* in the effluent, the procedure was the following:

The results from three bench-scale experiments completed to investigate PAA degradation in the wastewater effluent, done on the same day and using three different initial PAA concentrations, were plotted in **Erreur ! Source du renvoi introuvable.**. Using the following equation, the degradation was modelled in order to determine the k and D parameters.

$$ICT_{PAA} = \int_0^t (PAA_0 - D_{PAA}) e^{-k_{PAA}t} dt = \frac{PAA_0 - D_{PAA}}{k_{PAA}} (1 - e^{-k_{PAA}t})$$

*Equation A1*
*Source: Santoro et al., 2015*

The three k and D parameters found are in Table A 1.

*Table A 1. k and D parameters for the modelled degradation of PAA at the Venice WWTP*

| | *Test 1* | *Test 2* | *Test 3* | *Average* |
|---|---|---|---|---|
| *k* | 0.042555 | 0.0857298 | 0.081119 | 0.069801 |
| *D* | 0.006783 | 0.0022537 | 0.002334 | 0.003790 |

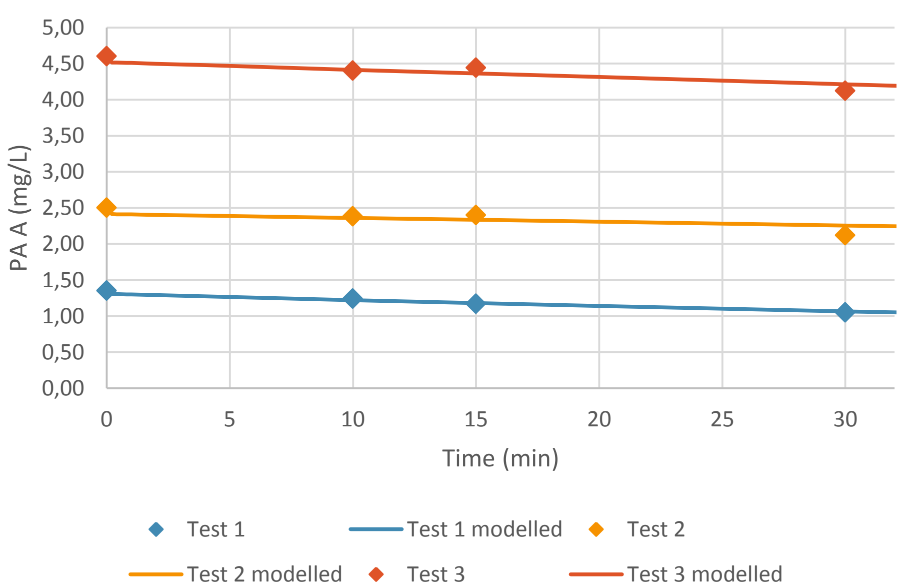



*Figure A 3. PAA degradation at the Venice WWTP*

Using the average k and D parameters found, ICTs were calculated for every dose and contact time provided by the treatment for the two months that the study covers. Following this, the ICTs were plotted as a function of log removal at the treatment plant. Then, a linear regression was used to predict the ICT for 3-log removal of *E. coli* at the Venice WWTP. Using the average contact time at the treatment plant, the dose of PAA needed for 3 log removal was calculated.

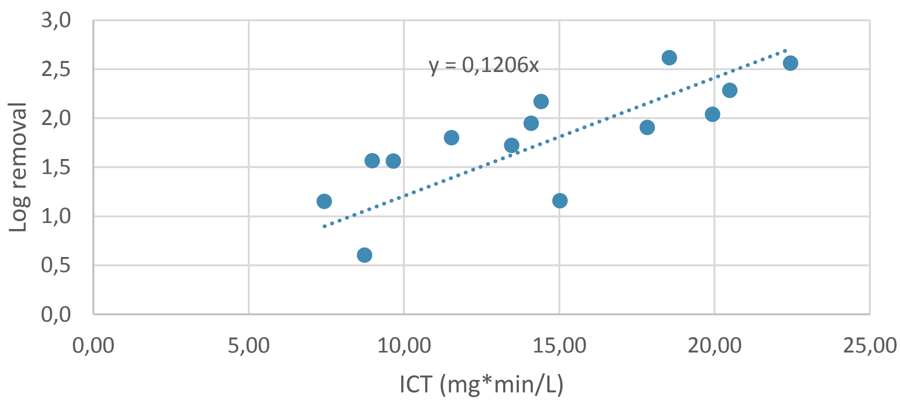



*Figure A 4. Calculated ICT as a function of log removal at the Venice WWTP.*

The contact time used was 19.4 minutes. Using Equation , the dose of PAA for 3 log removal of *E. coli* was found to be 2.35 mg/L and the residual 0.60 mg/L.

## Appendix C. Data sources, assumptions and process descriptions

*Table A 2. Data sources and process description for Venice WWTP*

| *Life cycle stage* | *Intermediate processes* | *Data source* | *Location* | *Comments* |
|---|---|---|---|---|
| *Pre-production* | Raw materials extraction | ecoinvent | - | Background process |
| *Chemicals production* | NaOCl production | ecoinvent | Europe | 15% solution state<br>Includes factory building and decommissioning, land occupation, electricity, heat and sodium hydroxide |
| | PAA production | Peroxychem | Europe | Includes chemicals necessary for PAA production: acetic acid, hydrogen peroxide, sodium hydroxide and sulfuric acid, chemical factory infrastructure, polyethylene for storage containers, all flows from ecoinvent. |
| | PFA on-site production | Venice WWTP | Europe | Includes hydrogen peroxide, formic acid and the DesinFix unit used for PFA production. |
| *Ancillary equipment production* | Pump production | ecoinvent | Europe | 40W pump, based on Grundfos UP 15-35x20 |
| | PFA Desinfix unit production | ecoinvent | Europe | Due to lack of information on the DesinFix unit, used the fictitious ecoinvent “building machine” as proxy, which contains only steel. |
| | Contact tank production | Venice WWTP | Europe | Estimated quantities of concrete and reinforcing steel based on the volume of water contained by the contact tank. Concrete and steel flows from ecoinvent. |
| | HDPE storage containers | Venice WWTP, Plastic Mart | Europe | Size on containers given by Venice WWTP, quantity of plastic estimated using Plastic Mart HDPE containers |
| *Transport* | Transportation of chemicals to the WWTP | ecoinvent | Europe | Includes vehicle operation, manufacturing and maintenance, as well as transport infrastructure (roads) construction, maintenance, operation and disposal. |
| *Disinfection* | Electricity | ecoinvent | Italy | Total calculated based on power of all equipment |
| | Chemical Residual | Venice WWTP | Italy | Calculated from the power consumption of equipment and average residual reported by the WWTP. |
| *Other* | All emissions to the environment from background processes | ecoinvent | | |

*Table A 3. Sources and process description for NW Langley WWTP*

| *Life cycle stage* | *Intermediate processes* | *Data source* | *Location* | *Comments* |
|---|---|---|---|---|
| *Pre-production* | Raw materials extraction | ecoinvent | | Background process |
| *Chemicals production* | NaOCl production | ecoinvent | North America | 15% solution state<br>Includes factory building and decommissioning, land occupation, electricity, heat and sodium hydroxide |
| | PAA production | Kemira Oyj | North | Includes chemicals necessary for PAA production: acetic acid, hydrogen |

| | | | | |
|---|---|---|---|---|
| | | | America | peroxide, sodium hydroxide and sulfuric acid, chemical factory infrastructure, polyethylene for storage containers, all flows from ecoinvent. |
| | Sodium hydrogen sulfite production | ecoinvent | North America | Includes raw materials, energy consumption, infrastructure and transports |
| *Ancillary equipment production* | Pump production | ecoinvent | North America | 40W pump, based on Grundfos UP 15-35x20 |
| | Contact tank production | Venice WWTP | North America | Estimated quantities of concrete and reinforcing steel based on the volume of water contained by the contact tank. Concrete and steel flows from ecoinvent. |
| | HDPE storage containers | Venice WWTP, Plastic Mart | North America | Size on containers given by Venice WWTP, quantity of plastic estimated using Plastic Mart HDPE containers |
| *Transport* | Transportation of chemicals to the WWTP | ecoinvent | North America | Includes vehicle operation, manufacturing and maintenance, as well as transport infrastructure (roads) construction, maintenance, operation and disposal. |
| *Disinfection* | Electricity | ecoinvent | British Columbia | Total calculated based on power of all equipment |
| | Chemical Residual | Venice WWTP | British Columbia | Calculated from the power consumption of equipment and average residual reported by the WWTP. |
| *Other* | All emissions to the environment from background processes | ecoinvent | | |

*Table A 4. Data and assumptions for the Venice WWTP*

| *Reference flow* | *Key parameters* | *Venice WWTP* | *Sources and Hypothesises* |
|---|---|---|---|
| *Storage tank (PAA)* | Lifespan<br>Volume<br>Quantity | 5 years<br>29 526 L<br>1 | Based on information from Plastic Mart, an HDPE storage container distributor. |
| *Storage tank (NaOCl)* | Lifespan<br>Volume<br>Quantity | 5 years<br>2 000 imp. gallons<br>1 x 567 kg | Based on published information from Watertanks.ca, storage tank distributor. |
| *DesinFix unit (PFA)* | Lifespan<br>Quantity | 10 years<br>1 | Used fictitious ecoinvent flow “building machine” created to represent a machine made of 100% steel and adapted to be more representative of the DesinFix unit. |
| *Transportation* | Distance | 1 000 km | All transport for the LCA is set to 1000 km for the baseline scenario. |
| *NaOCl* | Dose<br>Flow treated<br>Residual concentration | 2.79 mg/L<br>1141 $m^3$/hour | Based on the average dose calculated for the months of August and September of 2011.<br>Flow based on the average flow calculated for the months of September and August of 2006 (year PFA was used). Information provided by Asi SPA. |

| | | | |
|---|---|---|---|
| | Combined<br>Free | 0.62 mg/L<br>0.09 mg/L | |
| *PAA* | Dose<br>Flow treated<br>Residual concentration | 2.35 mg/L<br>1141 $m^3$/hour<br>0.16 mg/L | Dose calculated using the disinfection kinetics from bench scale experiments done at the treatment plant.<br>Residual calculated using the disinfection kinetics from bench scale experiments done at the treatment plant. |
| *PFA* | Dose<br>Flow treated<br>Residual concentration | 0.91 mg/L<br>1141 $m^3$/hour<br>252 kg | Based on the average dose calculated for the months of August and September of 2006<br>Flow based on the average flow calculated for the months of September and August of 2006. |
| *Pumps* | Lifespan<br>Quantity | 5 years<br>3 pumps with PAA<br>4 pumps with PFA<br>2 pumps with NaOCl | Used the ecoinvent pump as a proxy, due to lack of information on the actual pump used. Ecoinvent pump specifications (flow, voltage) are similar to pumps used for chemical dosing: Grundfos UP 15-35x20 with a capacity of 40W. |
| *Contact tank* | Lifespan | 30 years<br>53.45 $m^3$ of concrete<br>1 669 kg of steel | Due to limited information about the contact tank used in Venice, used the dimensions of the NW Langley contact tank and applied a factor due to slightly different sizes. |
| *Electricity* | Pump power<br>PAA<br>NaOCl<br>PFA<br>Cooling unit (PFA)<br>Time | 220 W<br>350 W<br>1.5 kW<br>1 464 hours (2 months) | Information on the sources of electricity specific to each location was obtained from the ecoinvent databased. |

*Table A 5. Data sources and assumptions for the NW Langley WWTP*

| *Reference flow* | *Key parameters* | *NW Langley WWTP* | *Sources and hypothesises* |
|---|---|---|---|
| *Storage tank (PAA)* | Lifespan<br>Volume<br>Quantity | 5 years<br>29 526 L<br>1 | Based on information from Plastic Mart, an HDPE storage container distributor. |
| *Storage tank (NaOCl)* | Lifespan<br>Volume<br>Quantity | 5 years<br>2 000 imp. gallons | Based on published information from Watertanks.ca, storage tank distributor, and Metro Vancouver |

| | | | |
|---|---|---|---|
| | | 1 | |
| *Storage tank (SBS)* | Lifespan<br>Volume<br>Quantity | 5 years<br>1 250 L<br>1 | Based on published information from Watertanks.ca and from Metro Vancouver |
| *Transportation* | Distance | 1 000 km | All transport for the LCA is set to 1000 km, sensitivity analysis will report the results for different distances. |
| *NaOCl* | Dose<br>Flow treated<br>Residual concentration<br>Before dechlorination<br>After dechlorination | 2.79 mg/L<br>1 264 $m^3$/hour<br><br>0.8 mg/L<br>>0.1 mg/L | Calculated from Metro Vancouver annual report (2012) |
| *PAA* | Dose<br>Flow treated<br>Residual concentration | 2.10 mg/L<br>1 264 $m^3$/hour<br>0.4 mg/L | Calculated from Metro Vancouver annual report (2014) |
| *SBS residual ($SO_3^{-2}$)* | Concentration | 2.99 mg/L | Calculated from Metro Vancouver annual report (2012) |
| *Pumps* | Lifespan<br>Quantity | 5 years<br>3 pumps with PAA<br>2 pumps with NaOCl | From Metro Vancouver |
| *Contact tank* | Lifespan<br>Amount of concrete<br>Amount of steel | 30 years<br>56.33 $m^3$<br>1 758 kg | Specific dimensions sent by Metro Vancouver. The amount of concrete and steel was estimated from the contact tank blueprint. |
| *Electricity* | Pump power<br>PAA<br>NaOCl<br>SBS<br>Time | <br>220 W<br>350 W<br>350 W<br>1 464 hours | From Metro Vancouver |

## Appendix D. Complete inventory analysis

*Table A 6. Complete inventory analysis based on ecoinvent for the Venice WWTP*

| ***Flow*** | **Category** | **Amount** | **Unit** | **Provider** | **Pedigree matrix** |
|---|---|---|---|---|---|
| | | ***NaOCl product system*** | | | |
| | | ***Contact tank*** | | | |
| ***Input*** | | | | | |
| *bisphenol A epoxy based vinyl ester resin \| bisphenol A epoxy based vinyl ester resin production - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 3 167.19 | kg | bisphenol A epoxy based vinyl ester resin production \| bisphenol A epoxy based vinyl ester resin \| cut-off, S - RER | 5;1;2;3;3 |
| *concrete, high exacting requirements \| concrete production, for building construction, with cement CEM II/A - RoW* | 239:Manufacture of non-metallic mineral products n.e.c./2395:Manufacture... | 53.45 | m3 | concrete production, for building construction, with cement CEM II/A \| concrete, high exacting requirements \| cut-off, S - RoW | 5;1;1;1;3 |
| *reinforcing steel \| reinforcing steel production - RER* | 241:Manufacture of basic iron and steel/2410:Manufacture of basic iron a... | 1 668.91 | kg | reinforcing steel production \| reinforcing steel \| cut-off, S - RER | 5;1;1;1;3 |
| *Transformation, from industrial area, built up* | Resource/land | 183.68 | m2 | | 1;1;1;1;1 |
| *Transformation, to pasture and meadow* | Resource/land | 183.68 | m2 | | 1;1;1;1;1 |
| | | ***FRP tank*** | | | |
| ***Input*** | | | | | |
| *bisphenol A epoxy based vinyl ester resin \| bisphenol A epoxy based vinyl ester resin production - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.421*567 | kg | bisphenol A epoxy based vinyl ester resin production \| bisphenol A epoxy based vinyl ester resin \| cut-off, S - RER | 5;2;1;3;3 |
| *chemical, organic \| market for chemical, organic - GLO* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.632*567 | kg | market for chemical, organic \| chemical, organic \| cut-off, S - GLO | 2;1;1;3;3 |
| *glass fibre \| glass fibre production - RER* | 231:Manufacture of glass and glass products/2310:Manufacture of glass an... | 0.632*567 | kg | glass fibre production \| glass fibre \| cut-off, S - RER | 2;2;1;3;3 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RER* | 492:Other land transport/4923:Freight transport by road | 567*1 000 | t*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RER | 1;1;1;3;3 |
| *waste mineral wool, for final disposal \| treatment of waste mineral wool, inert* | 382:Waste treatment and disposal/3821:Treatment | -29.8242 | kg | treatment of waste mineral wool, inert material landfill \| waste mineral wool, for final disposal \| cut-off, S - RoW | 2;1;1;3;3 |

| | | | | | |
|---|---|---|---|---|---|
| *material landfill - RoW* | and disposal of non-haza... | | | | |
| ***Output*** | | | | | |
| *FRP tank (1 item)* | | 1 | Item | | |
| | | ***NaOCl disinfection*** | | | |
| ***Input*** | | | | | |
| *electricity, medium voltage \| market for electricity, medium voltage - IT* | 351:Electric power generation, transmission and distribution/3510:Electr... | 28.8 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - IT | 5;1;1;1;3 |
| *NaOCl equipment* | | 1 | Item(s) | NaOCl equipment - IT | |
| *NaOCl residual (item)* | | 1 | Item(s) | NaOCl residual - IT | |
| *NaOCl Solution production* | | 4 656/0.10 | kg | NaOCl Solution production | 1;3;2;1;3 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RER* | 492:Other land transport/4923:Freight transport by road | 4 656/0.10 *1000 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RER | 1;1;1;3;3 |
| ***Output*** | | | | | |
| *NaOCl disinfection* | | 1 | Item(s) | | |
| | | ***NaOCl equipment*** | | | |
| *Contact tank NaOCl* | | 0.00557 | Item(s) | Contact tank NaOCl (V) - IT | 3;1;1;1;1 |
| *FRP tank (1 item)* | | 0.0334 | Item(s) | FRP tank (V) - IT | 3;1;1;1;2 |
| *HDPE 55 gal shipping containers* | | 41 945.95/208 | Item(s) | HDPE 55 gal shipping containers | 5;1;1;3;3 |
| *pump, 40W \| market for pump, 40W - GLO* | 281:Manufacture of general-purpose machinery/2812:Manufacture of fluid p... | 0.01671 | Item(s) | market for pump, 40W \| pump, 40W \| cut-off, S - GLO | 3;1;1;1;3 |
| ***Output*** | | | | | |
| *NaOCl equipment* | | | | | |
| | | ***NaOCl residual*** | | | |
| ***Output*** | | | | | |
| *Chloramine* | Emission to water/surface water | 1 028 | kg | | 1;2;2;1;1 |
| *Hypochlorous acid* | Emission to water/fresh water | 147 | kg | | 1;2;2;1;1 |
| *NaOCl residual (item)* | | 1 | Item(s) | | |
| | | ***NaOCl Solution production*** | | | |
| *chemical factory, organics \| chemical* | 429:Construction of | 4.00E-10 | Item(s) | | 5;1;2;3;5 |

| | | | | | |
|---|---|---|---|---|---|
| *factory construction, organics - RER* | other civil engineering projects/4290:Constructi on o... | | | | |
| *chlorine, gaseous \| market for chlorine, gaseous - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.128 | kg | | 2;3;2;3;3 |
| *electricity, medium voltage \| market for electricity, medium voltage - IT* | 351:Electric power generation, transmission and distribution/3510:Electr... | 0.028 15 | kWh | | 3;1;2;3;3 |
| *heat, district or industrial, natural gas \| market group for heat, district or industrial, natural gas - RER* | 351:Electric power generation, transmission and distribution/3510:Electr... | 1.048 8 | MJ | | 3;1;2;3;3 |
| *heat, district or industrial, other than natural gas \| market group for heat, district or industrial, other than natural gas - RER* | 351:Electric power generation, transmission and distribution/3510:Electr... | 0.585 4 | MJ | | 3;1;2;3;3 |
| *sodium hydroxide, without water, in 50% solution state \| market for sodium hydroxide, without water, in 50% solution state - GLO* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.153 | kg | | 2;3;2;3;3 |
| ***Output*** | | | | | |
| *Chloride* | Emission to water/surface water | 0.48 | kg | | |
| *NaOCl Solution production* | | 1 | kg | | |
| | | ***Peracetic Acid Product System*** | | | |
| | | ***HDPE storage container*** | | | |
| ***Input*** | | | | | |
| *polyethylene, high density, granulate \| polyethylene production, high density, granulate - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 122 | kg | polyethylene production, high density, granulate \| polyethylene, high density, granulate \| cut-off, S - RER | 2;1;1;3;3 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RER* | 492:Other land transport/4923:Freight transport by road | 1 000*122 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RER | 1;1;1;3;3 |
| ***Output*** | | | | | |

| | | | | | |
|---|---|---|---|---|---|
| *PAA HDPE storage container* | | 1 | Item(s) | | |
| | | ***HDPE shipping containers*** | | | |
| ***Input*** | | | | | |
| *polyethylene, high density, granulate \| polyethylene production, high density, granulate - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 10.4 | kg | polyethylene production, high density, granulate \| polyethylene, high density, granulate \| cut-off, S - RER | 1;1;2;3;3 |
| *transport, freight, lorry, unspecified \| transport, freight, lorry, all sizes, EURO6 to generic market for transport, freight, lorry, unspecified - RER* | 492:Other land transport/4923:Freight transport by road | 1 000*10.4 | kg*km | transport, freight, lorry, all sizes, EURO6 to generic market for transport, freight, lorry, unspecified \| transport, freight, lorry, unspecified \| cut-off, S - RER | 1;1;2;3;3 |
| ***Output*** | | | | | |
| *HDPE 55 gal shipping containers* | | 1 | Item(s) | | |
| | | ***PAA 15% solution production*** | | | |
| ***Input*** | | | | | |
| *acetic acid, without water, in 98% solution state \| market for acetic acid, without water, in 98% solution state - GLO* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.278 1 | kg | market for acetic acid, without water, in 98% solution state \| acetic acid, without water, in 98% solution state \| cut-off, S - GLO | 1;1;2;2;1 |
| *chemical factory, organics \| chemical factory construction, organics - RER* | 429:Construction of other civil engineering projects/4290:Constructi on o... | 4.00E-10 | Item(s) | chemical factory construction, organics \| chemical factory, organics \| cut-off, S - RER | 5;1;2;3;5 |
| *electricity, medium voltage \| market for electricity, medium voltage - IT* | 351:Electric power generation, transmission and distribution/3510:Electr... | 0.02 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - IT | 5;1;2;3;5 |
| *hydrogen peroxide, without water, in 50% solution state \| hydrogen peroxide production, product in 50% solution state - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.297 9 | kg | hydrogen peroxide production, product in 50% solution state \| hydrogen peroxide, without water, in 50% solution state \| cut-off, S - RER | 1;1;2;2;1 |
| *sulfuric acid \| sulfuric acid production - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.007 | kg | sulfuric acid production \| sulfuric acid \| cut-off, S - RER | 1;1;2;2;1 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RER* | 492:Other land transport/4923:Freight transport by road | 1 000 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RER | 1;1;2;3;3 |
| *Water, unspecified natural origin* | Resource/unspecified | 0.000 42 | m3 | | 5;1;2;3;2 |
| ***Output*** | | | | | |
| *PAA production (kg)* | | 1 | kg | | |

| | | | | | |
|---|---|---|---|---|---|
| | | ***PAA disinfection*** | | | |
| ***Input*** | | | | | |
| *electricity, medium voltage \| market for electricity, medium voltage - IT* | 351:Electric power generation, transmission and distribution/3510:Electr... | 96.624 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - IT | 5;1;2;2;2 |
| *PAA equipment* | | 1 | Item(s) | PAA equipment - IT | |
| *PAA production (kg)* | | 3 926/0.15 | kg | PAA 15% solution production (V) - IT | 1;2;2;1;1 |
| *PAA residual (V)* | | 1 | Item(s) | PAA residual (V) - IT | |
| ***Output*** | | | | | |
| *PAA disinfection* | | 1 | Item(s) | | |
| | | ***PAA equipment*** | | | |
| ***Input*** | | | | | |
| *Contact tank NaOCl* | | 0.005 57 | Item(s) | Contact tank NaOCl (V) - IT | 2;1;2;1;2 |
| *HDPE 55 gal shipping containers* | | 109 | Item(s) | HDPE 55 gal shipping containers | 3;1;2;2;2 |
| *PAA HDPE storage container* | | 0.016 71 | Item(s) | 5m3 HDPE storage container (V) - IT | 2;1;2;2;2 |
| *pump, 40W \| market for pump, 40W - GLO* | 281:Manufacture of general-purpose machinery/2812:Manufacture of fluid p... | 0.050 1 | Item(s) | market for pump, 40W \| pump, 40W \| cut-off, S - GLO | 3;2;2;3;3 |
| ***Output*** | | | | | |
| *PAA equipment* | | 1 | Item(s) | | |
| | | ***PAA residual*** | | | |
| ***Output*** | | | | | |
| *PAA residual (V)* | | 1 | Item(s) | | |
| *Peracetic acid* | Emission to water/fresh water | 1 002 | kg | | 1;2;2;1;1 |
| | | ***Performic acid*** | | | |
| | | ***PFA disinfection*** | | | |
| ***Input*** | | | | | |
| *electricity, medium voltage \| market for electricity, medium voltage - IT* | 351:Electric power generation, transmission and distribution/3510:Electr... | 2 330.69 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - IT | 2;1;2;2;2 |
| *PFA equipment* | | 1 | Item(s) | PFA equipment - IT | |
| *PFA residual* | | 1 | Item(s) | PFA residual - IT | |

| | | | | | |
|---|---|---|---|---|---|
| *Venice PFA Production* | | 1 595 | kg | Venice PFA Production | 1;2;2;1;1 |
| ***Output*** | | | | | |
| *PFA disinfection* | | 1 | Item(s) | | |
| | | ***PFA equipment*** | | | |
| ***Input*** | | | | | |
| *building machine \| building machine production - RER* | 282:Manufacture of special-purpose machinery/2824:Manufacture of machine... | 0.5*(1/10)*(61/365) | Item(s) | building machine production \| building machine \| cut-off, S - RER | 5;5;2;3;5 |
| *Contact tank NaOCl* | | 0.005 57 | Item(s) | Contact tank NaOCl (V) - IT | 5;1;2;3;2 |
| *HDPE 55 gal shipping containers* | | 29 | Item(s) | HDPE 55 gal shipping containers | 5;1;2;3;3 |
| *PAA HDPE storage container* | | 0.033 4 | Item(s) | 5m3 HDPE storage container (V) - IT | 2;1;2;3;2 |
| *pump, 40W \| market for pump, 40W - GLO* | 281:Manufacture of general-purpose machinery/2812:Manufacture of fluid p... | 0.066 8 | Item(s) | market for pump, 40W \| pump, 40W \| cut-off, S - GLO | 2;1;2;3;3 |
| ***Output*** | | | | | |
| *PFA equipment* | | 1 | Item(s) | | |
| | | ***PFA residual*** | | | |
| ***Output*** | | | | | |
| *Performic acid* | Emission to water/fresh water | 252.37 | kg | | 1;2;2;1;1 |
| *PFA residual* | | 1 | Item(s) | | |
| | | ***Formic acid solution*** | | | |
| ***Input*** | | | | | |
| *formic acid \| market for formic acid - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.8 | kg | market for formic acid \| formic acid \| cut-off, S - RER | 1;2;2;1;2 |
| *sulfuric acid \| sulfuric acid production - RER* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.15 | kg | sulfuric acid production \| sulfuric acid \| cut-off, S - RER | 1;2;2;1;2 |
| *Water (fresh water)* | Resource/in water | 0.05 | kg | | 1;2;2;1;2 |
| ***Output*** | | | | | |
| *Venice formic acid solution* | | 1 | kg | | |
| | | ***PFA production*** | | | |
| ***Input*** | | | | | |
| *hydrogen peroxide, without water, in 50%* | 201:Manufacture of | 3.49 | kg | hydrogen peroxide production, product in 50% solution | 1;2;2;1;2 |

| | | | | | |
|---|---|---|---|---|---|
| *solution state \| hydrogen peroxide production, product in 50% solution state - RER* | basic chemicals, fertilizers and nitrogen compounds, ... | | | state \| hydrogen peroxide, without water, in 50% solution state \| cut-off, S - RER | |
| *transport, freight, lorry, unspecified \| market for transport, freight, lorry, unspecified - GLO* | 492:Other land transport/4923:Freight transport by road | (3.49+3.14)* 1000 | kg*km | market for transport, freight, lorry, unspecified \| transport, freight, lorry, unspecified \| cut-off, S - GLO | 1;1;2;2;2 |
| *Venice formic acid solution* | | 3.14 | kg | Venice formic acid solution | |
| ***Output*** | | | | | |
| *Venice PFA Production* | | 1 | kg | | |

*Table A 7. Complete inventory analysis based on ecoinvent for the Venice WWTP*

***NaOCl product system***

***Contact tank***

***Input***

| ***Flow*** | **Category** | **Amount** | **Unit** | **Provider** | **Pedigree matrix** |
|---|---|---|---|---|---|
| *bisphenol A epoxy based vinyl ester resin \| bisphenol A epoxy based vinyl ester resin production - RoW* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 3 167.19 | kg | bisphenol A epoxy based vinyl ester resin production \| bisphenol A epoxy based vinyl ester resin \| cut-off, S - RoW | 2;5;1;3;2 |
| *concrete, high exacting requirements \| concrete production, for building construction, with cement CEM II/A - RoW* | 239:Manufacture of non-metallic mineral products n.e.c./2395:Manufacture... | 56.33 | m3 | concrete production, for building construction, with cement CEM II/A \| concrete, high exacting requirements \| cut-off, S - RoW | 5;1;1;1;3 |
| *reinforcing steel \| reinforcing steel production - RoW* | 241:Manufacture of basic iron and steel/2410:Manufacture of basic iron a... | 1 758 | kg | reinforcing steel production \| reinforcing steel \| cut-off, S - RoW | 5;2;1;1;3 |
| *Transformation, from industrial area, built up* | Resource/land | 15.24*12.7 | m2 | | 1;1;1;1;1 |
| *Transformation, to pasture and meadow* | Resource/land | 15.24*12.7 | m2 | | 1;1;1;1;1 |
| ***Output*** | | | | | |
| *Contact tank NaOCl* | | 1 | Item(s) | | |

***Dechlorination***

***Input***

| | | | | | |
|---|---|---|---|---|---|
| *electricity, medium voltage \| market for electricity, medium voltage - CA-BC* | 351:Electric power generation, transmission and distribution/3510:Electr... | 11 537 *(1/1.48) *(1/27.6) *0.22*2 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - CA-BC | 2;5;2;2;2 |
| *PAA HDPE storage container* | | (1/5) | Item(s) | PAA HDPE storage container - CA-BC | 5;1;2;2;2 |
| *pump, 40W \| market for pump, 40W - GLO* | 281:Manufacture of general-purpose machinery/2812:Manufac | (2/10)*6.18 | Item(s) | market for pump, 40W \| pump, 40W \| cut-off, S - GLO | 5;1;2;2;2 |

| | | | | | |
|---|---|---|---|---|---|
| | ture of fluid p... | | | | |
| *sodium hydrogen sulfite \| sodium hydrogen sulfite production - RoW* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 1.15E+04 | kg | sodium hydrogen sulfite production \| sodium hydrogen sulfite \| cut-off, S - RoW | 1;1;2;1;2 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RoW* | 492:Other land transport/4923:Freight transport by road | 1 000 *11 537 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RoW | 1;1;2;1;2 |
| ***Output*** | | | | | |
| *Dechlorination* | | 1 | Item(s) | | |
| | | | ***FRP tank*** | | |
| ***Input*** | | | | | |
| *bisphenol A epoxy based vinyl ester resin \| bisphenol A epoxy based vinyl ester resin production - RoW* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.421*567 | kg | bisphenol A epoxy based vinyl ester resin production \| bisphenol A epoxy based vinyl ester resin \| cut-off, S - RoW | 3;1;1;3;2 |
| *chemical, organic \| market for chemical, organic - GLO* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.632*567 | kg | market for chemical, organic \| chemical, organic \| cut-off, S - GLO | 3;1;1;3;4 |
| *glass fibre \| glass fibre production - RoW* | 231:Manufacture of glass and glass products/2310:Manufacture of glass an... | 0.632*567 | kg | glass fibre production \| glass fibre \| cut-off, S - RoW | 3;1;1;3;3 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RoW* | 492:Other land transport/4923:Freight transport by road | 567*1000 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RoW | 1;1;1;3;2 |
| *waste mineral wool, for final disposal \| treatment of waste mineral wool, inert material landfill - RoW* | 382:Waste treatment and disposal/3821:Treatment and disposal of non-haza... | -29.8242 | kg | treatment of waste mineral wool, inert material landfill \| waste mineral wool, for final disposal \| cut-off, S - RoW | 1;1;1;3;2 |
| ***Output*** | | | | | |
| *FRP tank (1 item)* | | 1 | Item(s) | | |
| | | | ***NaOCl disinfection*** | | |
| ***Input*** | | | | | |
| *Dechlorination* | | 1 | Item(s) | Dechlorination - CA-BC | |
| *electricity, medium voltage \| market for electricity, medium voltage - CA-BC* | 351:Electric power generation, transmission and distribution/3510:Electr... | 90 200 *(1/1.11) *(1/27.6) *0.22*2 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - CA-BC | 5;2;2;2;2 |
| *NaOCl equipment* | | 1 | Item(s) | NaOCl equipment-Langley - CA-BC | |
| *NaOCl residual-Langley* | | 1 | Item(s) | NaOCl residual-Langley - CA-BC | |
| *NaOCl Solution Production (Langley)* | | 9.02E+04 | kg | NaOCl Solution Production (Langley) | |
| *transport, freight, lorry 16-32 metric ton,* | 492:Other land | 1 000 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| | 2;1;2;2;2 |

| | | | | | |
|---|---|---|---|---|---|
| *EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RoW* | transport/4923:Freight transport by road | *90 200 | | transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RoW | |
| ***Output*** | | | | | |
| *NaOCl disinfection* | | 1 | Item(s) | | |
| | | ***NaOCl equipment*** | | | |
| ***Input*** | | | | | |
| *Contact tank NaOCl* | | (1/30) | Item(s) | Contact tank NaOCl - CA-BC | 3;1;2;1;2 |
| *FRP tank (1 item)* | | 10-Jan | Item(s) | FRP tank - CA-BC | 5;1;2;1;2 |
| *pump, 40W \| market for pump, 40W - GLO* | 281:Manufacture of general-purpose machinery/2812:Manufacture of fluid p... | (2/10)*6.18 | Item(s) | market for pump, 40W \| pump, 40W \| cut-off, S - GLO | 5;1;1;2;3 |
| ***Output*** | | | | | |
| *NaOCl equipment* | | 1 | Item(s) | | |
| | | ***NaOCl residual*** | | | |
| ***Output*** | | | | | |
| *Chloramine* | Emission to water/surface water | 0 | kg | | |
| *Hypochlorous acid* | Emission to water/fresh water | 0 | kg | | |
| *NaOCl residual-Langley* | | 1 | Item(s) | | |
| *Sulfur dioxide* | Emission to water/fresh water | 5 731.8 | kg | | 1;1;2;1;1 |
| | | ***NaOCl Solution Production (Langley)*** | | | |
| ***Input*** | | | | | |
| *chemical factory, organics \| chemical factory construction, organics - RoW* | 429:Construction of other civil engineering projects/4290:Construction o... | 4.00E-10 | Item(s) | | 5;5;1;3;5 |
| *chlorine, gaseous \| market for chlorine, gaseous - RoW* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.128 | kg | | 2;1;1;3;2 |
| *electricity, medium voltage \| market for electricity, medium voltage - CA-BC* | 351:Electric power generation, transmission and distribution/3510:Electr... | 0.028 15 | kWh | | 3;1;1;3;2 |
| *heat, district or industrial, natural gas \| market for heat, district or industrial, natural gas - RoW* | 353:Steam and air conditioning supply/3530:Steam and air conditioning su... | 1.048 8 | MJ | | 3;1;1;3;2 |
| *heat, district or industrial, other than* | 3530:Steam and air | 0.585 4 | MJ | | 3;1;1;3;2 |

| | | | | | |
|---|---|---|---|---|---|
| *natural gas \| market for heat, district or industrial, other than natural gas - RoW* | conditioning supply/3530a: Steam and air conditioning... | | | | |
| *sodium hydroxide, without water, in 50% solution state \| market for sodium hydroxide, without water, in 50% solution state - GLO* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.153 | kg | | 2;1;1;3;2 |
| ***Output*** | | | | | |
| *NaOCl Solution Production (Langley)* | | 1 | kg | | |
| | | ***PAA Product system*** | | | |
| | | ***PAA disinfection*** | | | |
| ***Input*** | | | | | |
| *electricity, medium voltage \| market for electricity, medium voltage - CA-BC* | 351:Electric power generation, transmission and distribution/3510:Electr... | 40 825 *(1/1.12) *(1/27.6) *0.22*2 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - CA-BC | 5;1;1;3;2 |
| *PAA equipment-Langley* | | 1 | Item(s) | PAA equipment-Langley - CA-BC | |
| *PAA production (kg)* | | 4.08E+04 | kg | PAA production (Langley) | 1;1;2;1;2 |
| *PAA residual-Langley* | | 1 | Item(s) | PAA residual-Langley - CA-BC | |
| ***Output*** | | | | | |
| *PAA disinfection* | | 1 | Item(s) | | |
| | | ***PAA equipment*** | | | |
| ***Input*** | | | | | |
| *Contact tank NaOCl* | | (1/30) | Item(s) | Contact tank NaOCl - CA-BC | 3;1;2;1;2 |
| *PAA HDPE storage container* | | (1/5) | Item(s) | PAA HDPE storage container - CA-BC | 3;1;2;1;3 |
| *pump, 40W \| market for pump, 40W - GLO* | 281:Manufacture of general-purpose machinery/2812:Manufacture of fluid p... | (2/10)*6.18 | Item(s) | market for pump, 40W \| pump, 40W \| cut-off, S - GLO | 5;2;1;3;3 |
| ***Output*** | | | | | |
| *PAA equipment-Langley* | | 1 | Item(s) | | |
| | | ***HDPE storage container*** | | | |
| ***Input*** | | | | | |
| *polyethylene, high density, granulate \| polyethylene production, high density, granulate - RoW* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 122 | kg | polyethylene production, high density, granulate \| polyethylene, high density, granulate \| cut-off, S - RoW | 5;1;1;3;2 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RoW* | 492:Other land transport/4923:Freight transport by road | 1 000*122 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RoW | 1;1;1;2;2 |

| | | | | | |
|---|---|---|---|---|---|
| ***Output*** | | | | | |
| *PAA HDPE storage container* | | 1 | Item(s) | | |
| | | ***PAA production*** | | | |
| ***Input*** | | | | | |
| *acetic acid, without water, in 98% solution state \| market for acetic acid, without water, in 98% solution state - GLO* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.278 1 | kg | market for acetic acid, without water, in 98% solution state \| acetic acid, without water, in 98% solution state \| cut-off, S - GLO | 1;1;1;1;1 |
| *chemical factory, organics \| chemical factory construction, organics - RER* | 429:Construction of other civil engineering projects/4290:Constructio n o... | 4.00E-10 | Item(s) | chemical factory construction, organics \| chemical factory, organics \| cut-off, S - RER | 5;1;1;3;4 |
| *electricity, medium voltage \| market for electricity, medium voltage - CA-BC* | 351:Electric power generation, transmission and distribution/3510:Electr... | 0.02 | kWh | market for electricity, medium voltage \| electricity, medium voltage \| cut-off, S - CA-BC | 5;2;1;3;5 |
| *hydrogen peroxide, without water, in 50% solution state \| hydrogen peroxide production, product in 50% solution state - RoW* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.297 9 | kg | hydrogen peroxide production, product in 50% solution state \| hydrogen peroxide, without water, in 50% solution state \| cut-off, S - RoW | 1;1;1;1;1 |
| *sulfuric acid \| sulfuric acid production - RoW* | 201:Manufacture of basic chemicals, fertilizers and nitrogen compounds, ... | 0.007 | kg | sulfuric acid production \| sulfuric acid \| cut-off, S - RoW | 1;1;1;1;1 |
| *transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 - RoW* | 492:Other land transport/4923:Freight transport by road | 1 000 | kg*km | transport, freight, lorry 16-32 metric ton, EURO5 \| transport, freight, lorry 16-32 metric ton, EURO5 \| cut-off, S - RoW | 1;1;1;3;2 |
| *Water, unspecified natural origin* | Resource/unspecified | 0.000 42 | m3 | | 1;1;1;1;1 |
| ***Output*** | | | | | |
| *PAA production (kg)* | | 1 | kg | | |
| | | ***PAA residual-Langley*** | | | |
| ***Output*** | | | | | |
| *Peracetic acid* | Emission to water/fresh water | 1 959.6 | kg | | 1;2;2;1;1 |

## Appendix E. Characterisation factors for USEtox

In order to calculate the missing characterisation factors, the USEtox model, available for download at usetox.org was used.

Model inputs are described in Table A 8.

*Table A 8. USEtox model inputs for the $SO_2$ characterisation factor*

| | *Units* | | *Source* |
|---|---|---|---|
| *Name* | Sulfur dioxide | | |
| *MW* | $g.mol^{-1}$ | 64.06 | National Center for Biotechnology and Information (2017) |
| *pKa.gain* | - | 6.97 | |
| *pKa.loss* | - | 1.9 | |
| $K_{OW}$ | $L.L^{-1}$ | 0.213 796 209 | |
| *Koc* | $L.kg^{-1}$ | 0.360 827 808 | Trapp (2017) |
| $K_H 25C$ | $Pa.m^{3}\cdot mol^{-1}$ | 83.333 333 33 | National Institute of Standards and Technology (2017) |
| *Pvap25* | Pa | 324 240 | National Center for Biotechnology and Information (2017) |
| *Sol25* | $mg.L^{-1}$ | 87 471.58 | |
| $K_{DOC}$ | $L.kg^{-1}$ | 0.0171 036 97 | |
| $Kp_{SS}$ | $L.kg^{-1}$ | 1.531 023 498 | Calculated with USEtox |
| $Kp_{Sd}$ | $L.kg^{-1}$ | 0.765 511 749 | |
| $Kp_{Sl}$ | $L.kg^{-1}$ | 0.013 793 569 | |
| $kdeg_A$ | $s^{-1}$ | 6.49 961E-08 | |
| *kOH* | $cm^3/mol/s$ | 1.30E-12 | Atkinson, R.; et al. (2004) |
| $kdeg_W$ | $s^{-1}$ | 0.000 000 53 | US EPA (2012) |
| $kdeg_{Sd}$ | $s^{-1}$ | 0.000 000 265 | Calculated with USEtox |
| $kdeg_{Sl}$ | $s^{-1}$ | 7.221 79E-09 | |
| $av_{logEC50}$ | $log(mg.L^{-1})$ | 1.514 737 546 | British Oxygen Company (2011) |

*Table A 9. USEtox model inputs for the PFA characterisation factor*

| | *Units* | | *Source* |
|---|---|---|---|
| *Name* | Performic acid | | |
| *MW* | $g.mol^{-1}$ | 62.03 | National Center for Biotechnology and Information (2017) |
| *pKa.loss* | - | 7.77 | |
| $K_{OW}$ | $L.L^{-1}$ | 0.023 988 329 | |
| *Koc* | $L.kg^{-1}$ | 0.009 835 215 | US EPA (2017) |
| $K_H 25C$ | $Pa.m^{3}\cdot mol^{-1}$ | 0.192 | |

| | | | |
|---|---|---|---|
| *Pvap25* | Pa | 10 000 | |
| *Sol25* | $mg.L^{-1}$ | 1 000 000 | |
| *$kdeg_A$* | $s^{-1}$ | 0.000 003 | |
| *kOH* | $cm^3/mol/s$ | | |
| *$kdeg_W$* | $s^{-1}$ | 0.000 000 53 | |
| *$kdeg_{Sd}$* | $s^{-1}$ | 0.000 000 265 | |
| *$kdeg_{Sl}$* | $s^{-1}$ | 5.888 89E-08 | |
| *$av_{logEC50}$* | $log(mg.L^{-1})$ | -0.77 | Chhetri et al. (2014) |
| *$BAF_{fish}$* | $L.kg_{fish}^{-1}$ | 0.894 | US EPA (2017) |

*Table A 10. USEtox model inputs for the PAA characterisation factor*

| | *Units* | | *Source* |
|---|---|---|---|
| *Name* | | Peracetic acid | |
| *PesticideTargetClass* | - | Fungicide, Nematicide, Microbiocide | |
| *PesticideChemClass* | - | Other pesticide class | |
| *MW* | $g.mol^{-1}$ | 76.05 | |
| *pKaChemClass* | - | acid | |
| *pKa.loss* | - | 7.83 | |
| *$K_{OW}$* | $L.L^{-1}$ | 0.085 113 804 | |
| *Koc* | $L.kg^{-1}$ | 0.034 896 66 | |
| *$K_H25C$* | $Pa.m^3.mol^{-1}$ | 0.216 14 | |
| *Pvap25* | Pa | 1933.333 333 | |
| *Sol25* | $mg.L^{-1}$ | 1 000 000 | |
| *$kdeg_A$* | $s^{-1}$ | 3.031 62E-06 | US EPA (2017) |
| *kOH* | $cm^3/mol/s$ | 4E-12 | |
| *$kdeg_W$* | $s^{-1}$ | 5.348 36E-07 | |
| *$kdeg_{Sd}$* | $s^{-1}$ | 5.942 62E-08 | |
| *$kdeg_{Sl}$* | $s^{-1}$ | 2.674 18E-07 | |
| *$kdiss_P$* | $s^{-1}$ | 6.839 77E-06 | |
| *$kdiss_{wheat}$* | $s^{-1}$ | 1.035 24E-05 | |
| *$kdiss_{rice}$* | $s^{-1}$ | 5.188 49E-06 | |
| *$kdiss_{tomato}$* | $s^{-1}$ | 7.328 94E-06 | |
| *$kdiss_{apple}$* | $s^{-1}$ | 5.821 58E-06 | |
| *$kdiss_{lettuce}$* | $s^{-1}$ | 1.462 32E-05 | |
| *$kdiss_{potato}$* | $s^{-1}$ | 1.161 56E-05 | |
| *$av_{logEC50}$* | $log(mg.L^{-1})$ | -0.16 | Chhetri et al. (2014) |
| *$BAF_{fish}$* | $L.kg_{fish}^{-1}$ | 0.896 39 6186 | US EPA (2017) |

*Table A 11. USEtox model inputs for the HOCl characterisation factor*

| | Units | | Source |
|---|---|---|---|
| *Name* | Hypochlorous acid | | National Center for Biotechnology and Information (2017) |
| *MW* | $g.mol^{-1}$ | 52.46 | |
| *pKa.loss* | - | 7.53 | |
| $K_{OW}$ | $L.L^{-1}$ | 1.348 962 883 | Céondo GmbH (2017) |
| *Koc* | $L.kg^{-1}$ | 0.553 074 782 | Calculated with USEtox |
| $K_H 25C$ | $Pa.m^{3}.mol^{-1}$ | 0.153 526 347 | National Institute of Standards and Technology (2017) |
| $kdeg_A$ | $s^{-1}$ | 0.000 000 375 | Calculated with USEtox |
| *kOH* | $cm^3/mol/s$ | | Atkinson et al. (2007) |
| $kdeg_W$ | $s^{-1}$ | 0.000 000 53 | US EPA (2017) |
| $kdeg_{Sd}$ | $s^{-1}$ | 0.000 000 265 | Calculated with USEtox |
| $kdeg_{Sl}$ | $s^{-1}$ | 5.888 89E-08 | Calculated with USEtox |
| $av_{logEC50}$ | $log(mg.L^{-1})$ | -1.11 | |

## Appendix F. Breakdown of chemical production potential impacts based on production of 1 kg of active substance

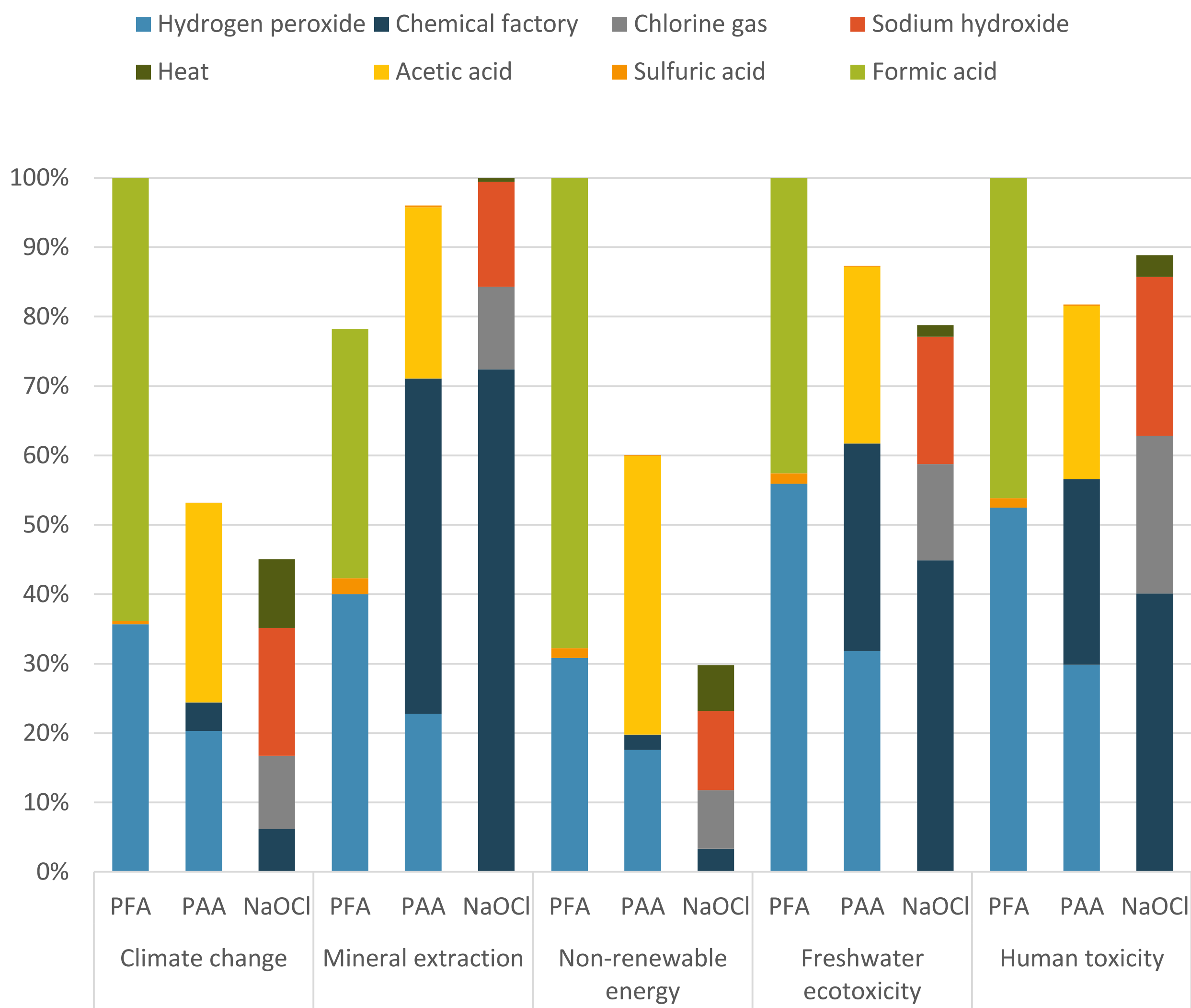



*Figure A 5. Breakdown of the potential impacts of chemical production*

## Appendix G. Sensitivity analysis on contact tank

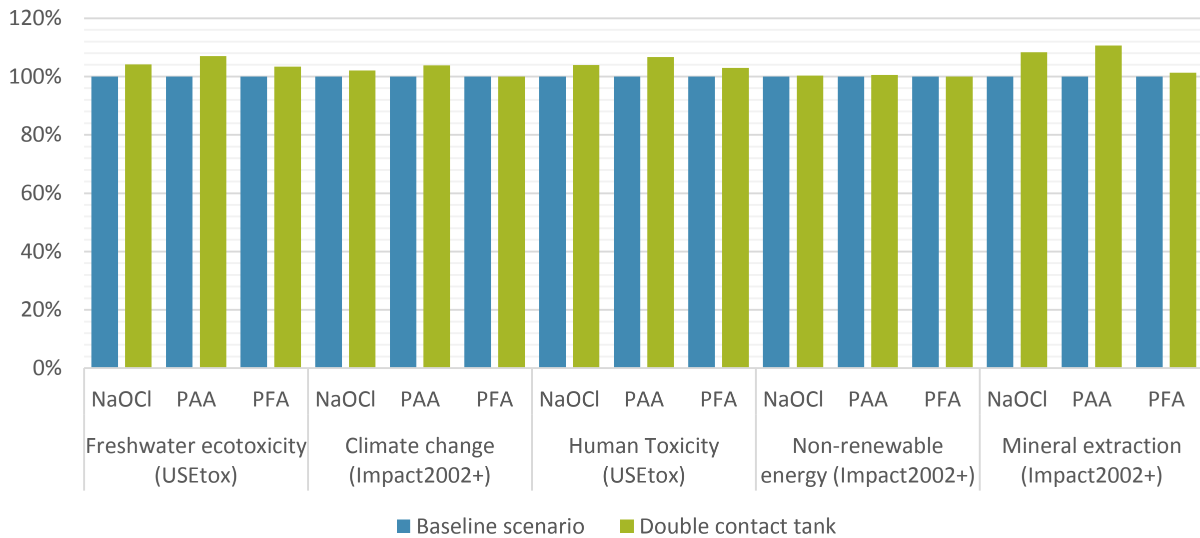



*Figure A 6. Increase in total potential impacts of **equipment** at the Venice WWTP when contact tank is doubled in size*

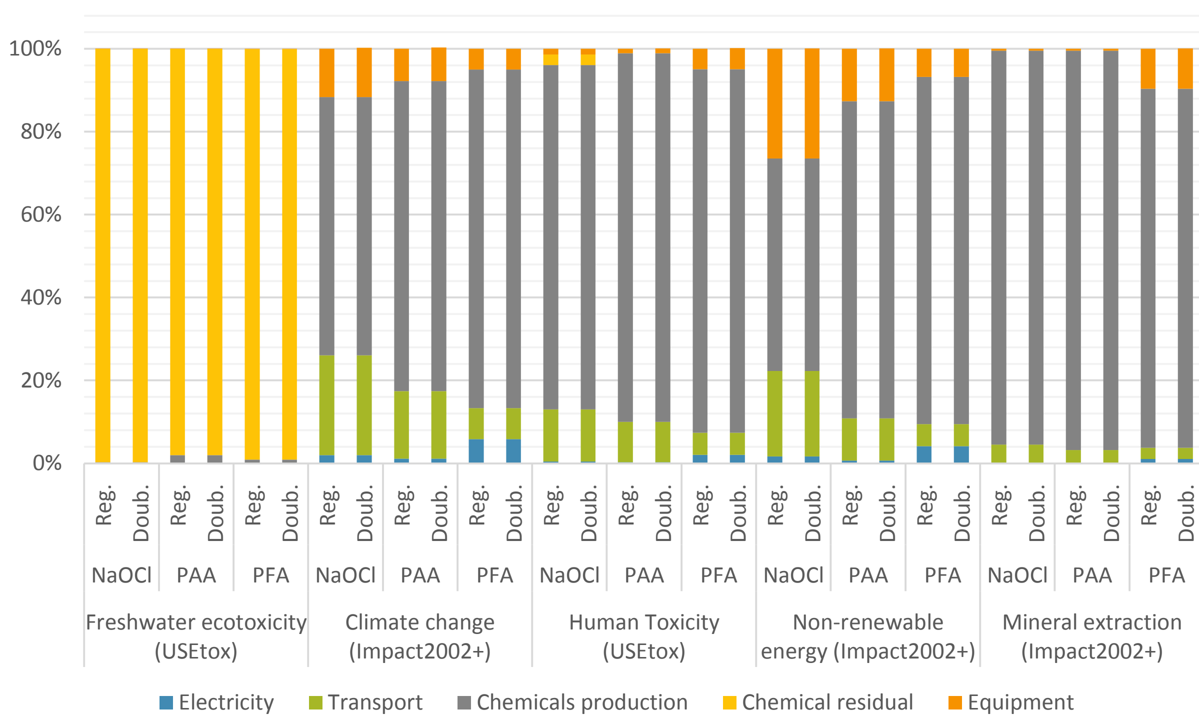



*Figure A 7. Increase in **total potential impacts** at the Venice WWTP when contact tank is doubled in size*

# Appendix H. Data quality evaluation

*Table A 12. Data quality indicators with five levels of quality as described in a pedigree matrix*

| *Quality score* | *1* | *2* | *3* | *4* | *5* |
|---|---|---|---|---|---|
| *Reliability* | Verified data based on measurements | Verified data partially based on measurements or non-verified data based on measurements | Non-verified data partially based on qualified estimates | Qualified estimates (e.g., by expert) | Non-qualified estimate |
| *Completeness* | Representative data from all sites relevant for the market considered, over an adequate period to even out normal fluctuations | Representative data from >50% of the sites relevant for the market considered, over an adequate period to even out normal fluctuations | Representative data from only some sites (<50%) relevant for the market considered or from >50% of sites but from shorter periods | Representative data from only one site relevant for the market considered or from some sites but from shorter periods | Representativeness unknown or data from a small number of sites and from shorter periods |
| *Temporal correlation* | Less than 3 years of difference to the time period of the data set | Less than 6 years of difference to the time period of the data set | Less than 10 years of difference to the time period of the data set | Less than 15 years of difference to the time period of the data set | Age of data unknown or more than 15 years of difference to the time period of data set |
| *Geographical correlation* | Data from area under study | Average data from larger area with similar production conditions | Data from area with similar production conditions | Data from area with slightly similar production conditions | Data from unknown area or distinctly different area (North America instead of Middle-East) |
| *Further technological correlation* | Data from enterprises, processes, and materials under study | Data from processes and materials under study, but from different enterprises | Data from processes and materials under study but from different technology | Data on related processes or materials | Data on related processes on laboratory scale or from different technology |
| *Sample size* | >100, continuous measurements | >20 | >10 | >=3 | Unknown |

*Source: Ciroth, A. et al. 2013. International Journal of Life Cycle Assessment*

*Table A 13. Default uncertainty factors (contributing to the square of the geometric standard deviation) applied to the quality matrix*

| *Indicator score* | | *1* | *2* | *3* | *4* | *5* |
|---|---|---|---|---|---|---|
| *Reliability* | $U_R$ | 1.00 | 1.05 | 1.10 | 1.20 | 1.50 |
| *Completeness* | $U_C$ | 1.00 | 1.02 | 1.05 | 1.10 | 1.20 |
| *Temporal correlation* | $U_T$ | 1.00 | 1.03 | 1.10 | 1.20 | 1.50 |
| *Geographical correlation* | $U_G$ | 1.00 | 1.01 | 1.02 | - | 1.10 |
| *Further technological correlation* | $U_L$ | 1.00 | - | 1.20 | 1.50 | 2.00 |
| *Sample size* | $U_S$ | 1.00 | 1.02 | 1.05 | 1.10 | 1.20 |

*Source: Frischknecht, R. et al., 2004. International Journal of Life Cycle Assessment, 10, 3–9.*

# Appendix I. Monte Carlo simulations

## Venice WWTP

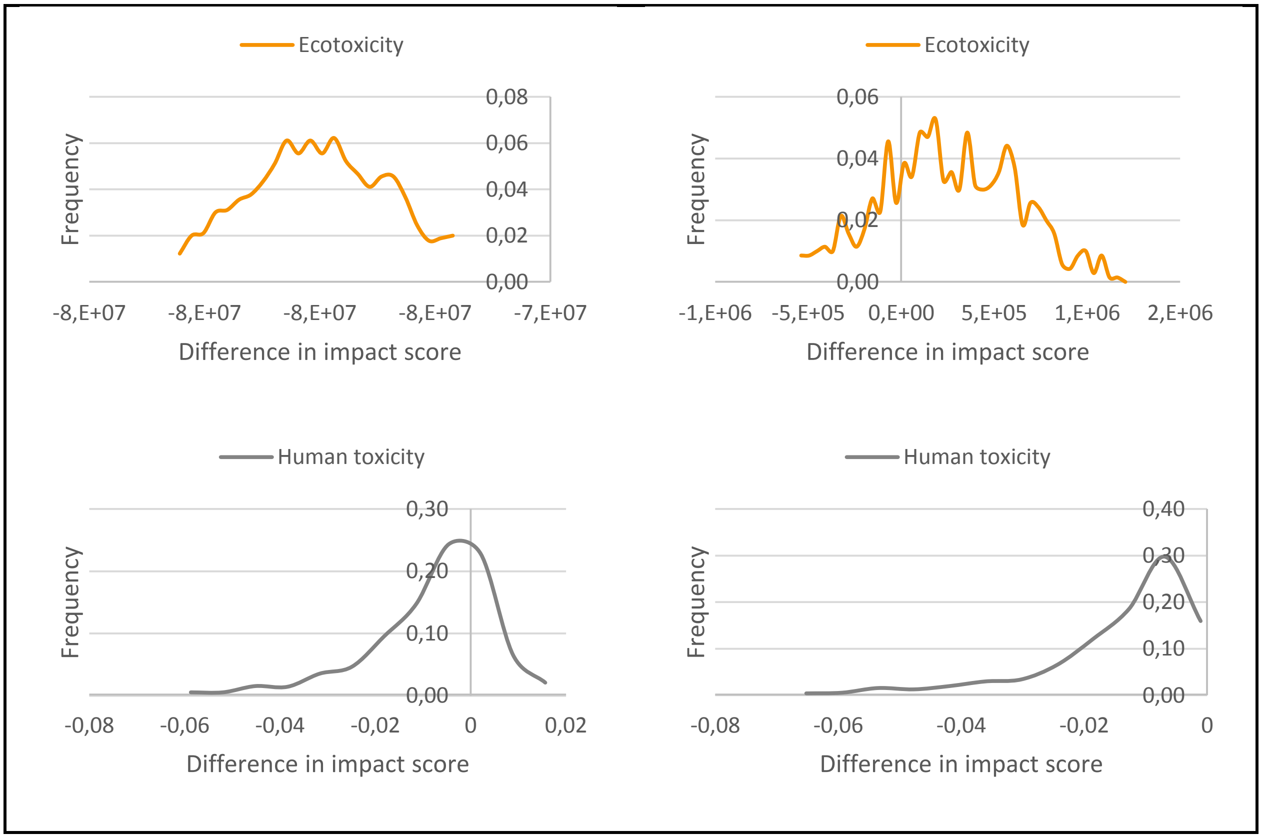
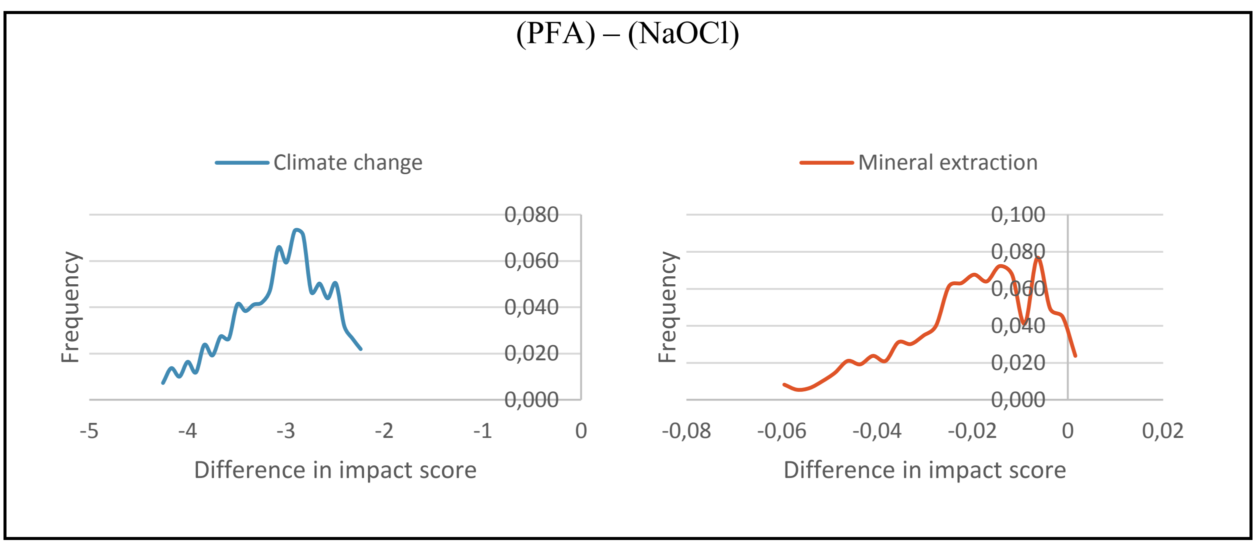



*Figure A 8. Monte Carlo analysis on the difference in impacts between NaOCl and PAA, and PAA and PFA product systems at the Venice WWTP*

## NW Langley WWTP



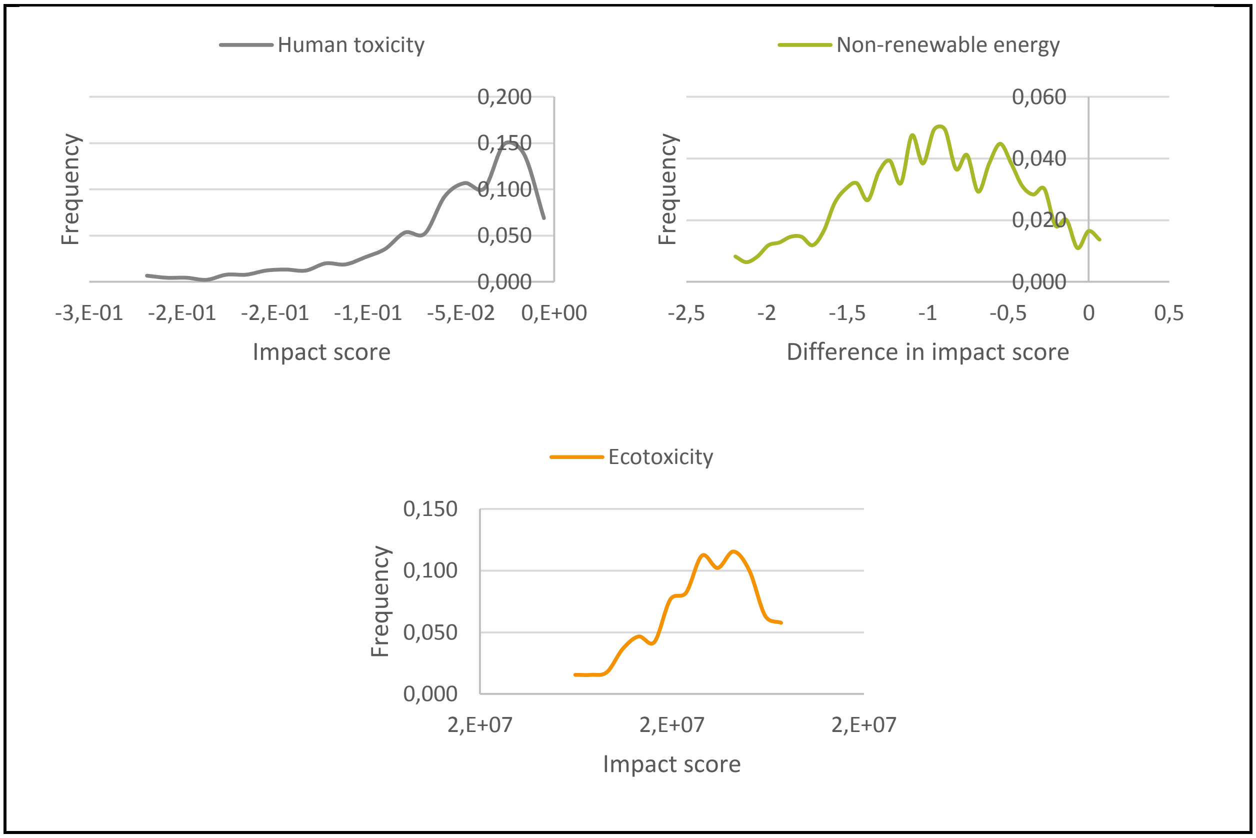



*Figure A 9. Monte Carlo analysis on the difference in impacts between NaOCl and PAA product systems at the NW Langley WWTP*