



Guideline for monitoring water quality and management of disinfection by-products in drinking water distribution networks.

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Abstract

This deliverable presents an integrated approach for monitoring water quality and managing disinfection by-products (DBPs) in drinking water distribution networks (DWDNs), addressing challenges linked to both pipe repair interventions and routine system operation.

Ensuring safe drinking water in Europe requires balancing effective disinfection with the control of DBPs, which may pose risks to human health. This challenge is further compounded by infrastructure ageing and rehabilitation practices, such as pipe relining, which can introduce additional contaminants through material leaching. These pressures are expected to intensify under climate change, requiring more proactive and risk-based management strategies.

The deliverable first identifies key contaminants released from materials in contact with water, including bisphenols, amines, chlorophenols, and nitrosamines, and evaluates their role as DBP precursors. A case study in Milan (CS#2) shows that pipe relining can lead to temporary increases in organic matter and DBP formation, particularly during the initial phase of operation. While flushing procedures effectively reduce contamination, certain compounds, especially nitrosamines, may persist and require continued monitoring. These results support the definition of targeted monitoring strategies, including appropriate parameters, sampling frequency, and complementary indicators such as total organic carbon and toxicity.

An integrated human health risk assessment framework was developed, considering both direct exposure through drinking water and indirect exposure via consumption of home-grown vegetables. Experimental results indicate that some contaminants, particularly nitrosamines, can be taken up by plants, contributing to overall exposure. The assessment shows that risk thresholds may be exceeded even at low concentrations, highlighting the need for improved analytical sensitivity and a broader perspective on exposure pathways.

In addition, a water management tool was developed to support decision-making in DBP minimization. The tool combines hydraulic modelling, DBP prediction, and risk assessment, and introduces a normalized risk index (NRI) to provide an intuitive evaluation of health risks across the network. Its application to a real system in Tarragona (CS#3) demonstrates its ability to identify spatial and seasonal variations in DBP-related risks, supporting targeted operational actions.

Overall, this work provides practical methodologies and tools to support water utilities in transitioning towards proactive, risk-based management of drinking water systems. The proposed approach contributes to safer and more resilient water supply under evolving environmental and regulatory conditions.



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Abbreviations

Acronym	Description	Acronym	Description
2-EHGE	2-ethylhexyl glycidyl ether	NP	Nonylphenol
ADD	Average Daily Dose	NRI	Normalized Risk Index
AT	Averaging time	PAH	Polycyclic aromatic hydrocarbons
BADGE	BPA-diglycidylether	PB	Polybutene
BaP	Benzo[a]pyrene	PE	Polyethylene
BDCM	Bromodichloromethane	PEX	Crosslinked polyethylene
BPA	Bisphenol A	PFOA	Perfluorooctanoic acid
BPF	Bisphenol F	PP	Polypropylene
Br ₂ MSA	Dibromomethanesulfonic acid	PVC	Polyvinyl chloride
BW	Body weight	RfD	Reference dose
Cl ₂ MSA	Dichloromethanesulfonic acid	SF	Slope factor
CS	Case Study	TCAA	Trichloroacetic acid
DBAA	Dibromoacetic acid	TCM	Trichloromethane (chloroform)
DBCM	Dibromochloromethane	TDI	Tolerable daily intake
DBP	Disinfection by-product	TBM	Tribromomethane (bromoform)
DCAA	Dichloroacetic acid	THMs	Trihalomethanes
DOC	Dissolved organic carbon	TOC	Total organic carbon
DWDN	Drinking Water Distribution Network	TOX	Total halogenated organic compounds
DWTP	Drinking Water Treatment Plant	TTHMs	Total trihalomethanes
EBT	Effect-based threshold	US-EPA	United States Environmental Protection Agency
ED	Exposure duration	UVA254	Ultraviolet absorbance at 254 nm
EF	Exposure frequency	VF	Volatilization factor
EFSA	European Food Safety Authority	VOCs	Volatile organic compounds
ET	Exposure time		
ETBE	Ethyl tert-butyl ether		
GAC	Granular activated carbon		
HAAs	Haloacetic acids		
HANs	Haloacetonitriles		
HQ	Hazard quotient		
ILCR	Increased lifetime cancer risk		
IR	Ingestion rate		
LOD	Limit of detection		
LOQ	Limit of quantification		
MBAA	Monobromoacetic acid		
MCAA	Monochloroacetic acid		
MTBE	Methyl tert-butyl ether		
N-DBP	Nitrogenous disinfection by-product		
NDMA	N-nitrosodimethylamine		
NMOR	N-nitrosomorpholine		



1. Introduction

Access to safe drinking water is a fundamental prerequisite for public health and societal well-being. While drinking water treatment effectively prevents the transmission of waterborne diseases, the use of chemical disinfectants can unintentionally lead to the formation of disinfection by-products (DBPs).

Since their first identification in the 1970s, several thousand DBPs have been reported in disinfected drinking water. Among these, trihalomethanes (THMs) and haloacetic acids (HAAs) are the most prevalent and extensively regulated compounds. Other DBP families, such as nitrogenous and aromatic DBPs, are typically detected at lower concentrations but often exhibit higher toxicity, including mutagenic, genotoxic, or carcinogenic effects. As a result, regulatory frameworks worldwide impose increasingly stringent limits on selected DBPs, placing significant pressure on water utilities to ensure compliance while maintaining microbiological safety.

The formation and fate of DBPs in DWDNs depend on a complex interplay of factors, including the type and dose of disinfectant, source water quality, natural organic matter (NOM) characteristics, presence of inorganic species such as bromide, hydraulic residence time, and operational conditions within the distribution system. Unlike treatment plants, distribution networks are dynamic and spatially heterogeneous systems, where water quality continues to evolve due to prolonged disinfectant contact times, variable flows, storage tanks, and secondary disinfection practices. Consequently, DBP formation may persist or even increase after water leaves the treatment plant, making their control particularly challenging.

Several strategies have been proposed to mitigate DBP formation, including precursor removal during treatment, optimization of disinfectant type and dose, reduction of water residence time, and implementation of additional treatment processes prior to consumption. However, these measures often involve trade-offs between microbiological protection, chemical risk, operational complexity, and cost. In this context, the management of DBPs represents a critical scientific, technical, and regulatory challenge with direct implications for public health and water utility operations.

On the other hand, during transport, several events may occur that potentially contaminate water, such as leaching of chemicals from materials in contact with water and DBPs formation. The pipe materials can be very different, ranging from metals, polymers or cement: this results in a wide range of possible contaminants leaching, either inorganic or organic. In addition, the need to renovate aged pipelines raised interest for relining, especially in densely populated urban areas to minimize working sites: an inner layer is created by polymerization of epoxy resins, adding another source of leaching. If a residual disinfectant is present, the formation of additional DBPs from leached chemicals must be taken into account.

Hence, designing targeted monitoring campaigns and developing models and tools to control DBP formation is crucial to ensure safe drinking water to consumers, while comprehensively accounting for all possible exposure routes to chemicals and DBPs.

This deliverable covers two key aspects of DWDN management: network monitoring after pipe repairs (Chapter 3), and the routine decision-making process for minimizing DBPs by providing utilities with the necessary knowledge and tools (Chapter 4).



2. Objectives

The objectives of this deliverable are divided into the two key aspects covered: network monitoring after pipe repairs and water management tool for minimizing DBPs.

Objectives related to network monitoring after pipe repairs:

1. Outlining potential criticalities related to water contamination due to the release of constituents in materials in contact with water, supporting the selection of chemical compounds to be monitored (addressed stakeholders: policymakers, water utilities).
2. Supporting the definition of monitoring campaigns in terms of parameters, frequency and sampling location when relining is adopted, based on data collected from Task 3.1 (CS#2, Milan) (addressed stakeholders: water utilities).
3. Proposing an experimental protocol to evaluate potential contaminants uptake in home-grown vegetables (addressed stakeholders: researchers), using sprouts as reference.
4. Proposing a framework to assess human health risk due to the exposure to contaminated water, through direct water ingestion and ingestion of home-grown vegetables (addressed stakeholders: policymakers).

Objectives related to the water management tool for minimizing DBPs in DWDNs:

1. Development of a water management tool based on DBP concentration estimation and associated human health risk assessment.
2. Definition of the conditions for the implementation and use of the water management tool.
3. Definition of a set of recommendations for water management in DWDNs
4. Development of a simplified online tool for the preliminary evaluation of DBP distribution in the network and the associated human health risk.



3. Network monitoring after pipe repairs

This section contains the following information: (i) literature review of the critical contaminants released from materials in contact with water, including materials used for relining; (ii) design of the monitoring campaign in a drinking water treatment plant (DWTP) in CS#2 and analysis of the data collected; (iii) lab experiments on vegetable uptake in two types of sprouts, (iv) assessment of human health risk through apportioning the risk among the contaminants and the exposure routes, and (v) final recommendations for utilities.

3.1. Literature review

DWDNs, intended as the complex network of pipes and accessories as valves, gaskets and sealing rings, comprise a wide range of materials, from metals, potentially inner-coated by inorganic (e.g. cement mortar) or organic (e.g. epoxy-resins) layers, to cement, rubber and polymers (e.g. PVC, PE, PEX, PP, HDPE). Materials in contact with water undergo degradation due to water aggressiveness, biofilm formation and the action of disinfectants, thus requiring periodical restoration. Recently, relining techniques have gained interest, as they allow pipe repair by creating a new inner layer through on-site resin polymerization. All these materials, regardless of their age, may leach chemicals that can be toxic and/or react with residual disinfectants, leading to the formation of DBPs, which may also be toxic.

Concerning metal pipes, lead was one of the first materials used for DWDNs (Stefan et al., 2023), representing the main source of lead in drinking water, whose leaching occurs through the formation of corrosion scales (Kim & Herrera, 2010). Moreover, the produced scales can react with chlorine-based disinfectants leading to further oxidation. However, lead can originate also from the zinc coating itself (Clark et al., 2015). Another material used in the past is copper, which is also subjected to corrosion and scale formation (Merkel & Pehkonen, 2006). Copper in contact with water is usually oxidized by dissolved oxygen to copper ions, which can generate different types of precipitates depending on water chemistry (D. J. G. Ives & A. E. Rawson, 1962; Lagos et al., 2001). Moreover, the presence of chlorine-based disinfectants proved to enhance corrosion (Hong & Macauley, 1998). Concerning iron, different options are used for drinking water: cast iron, galvanized iron, unlined cast iron and line ductile iron (Stefan et al., 2023). Iron release is due to progressive corrosion, formation of scales and dissolution, favored by the presence of oxidants, such as dissolved oxygen and residual disinfectants, and water characteristics, such as hardness, nitrate and pH (Sarin et al., 2004; Zhang et al., 2020; Lin et al., 2021). Moreover, it was found that biofilm attached to iron scales reacted with NaClO resulting in N-DBPs formation (Qi et al., 2022). Iron release from corroded pipes is one of the main causes of “colored waters” problems (Sarin et al., 2004). Regarding steel, as reported for the other metals, corrosion by dissolved oxygen in water or by residual disinfectants plays an important role (Cox & Roetheli, 1931; Giovanardi et al., 2020), leading to the release of a range of metals into drinking water, primarily iron, calcium, manganese, zinc and lead from corrosion scales (Tian et al., 2021). It was found that high pH, alkalinity and the presence of orthophosphate might reduce leaching; on the other hand, chloride and sulphate promote the re-release of metals, as well as prolonged stagnation times.

Cement has been extensively used for pipe manufacturing (Stefan et al., 2023). This material, in the late 1920s was mixed with asbestos to create composites that were used worldwide for water mains in DWDNs (Liu et al., 2022; Zavašnik et al., 2022). Cement mortar, made of water, cement and sand, is also used for lining purposes (Zavašnik et al., 2022). Over the years, studies outlined that cements and



cement-composites release multiple substances, depending on water and pipe characteristics, operating conditions, such as maintenance and repairs, and the presence of residual disinfectants (chlorine-based disinfectants), which enhance corrosion (Zavašnik et al., 2022). Calcium, silica, aluminum, cadmium, chromium and lead can be leached from cement-based pipes (Bielski et al., 2020; Zielina et al., 2022; Stefan et al., 2023), together to asbestos fibers due to asbestos-cement pipe ageing (Stefan et al., 2023). A monitoring study in New Zealand reported an average concentration of long asbestos fibers of 0.9 MFL (millions of asbestos fibers per liter), with an extreme value of 56 MFL, exceeding the regulatory limit of 7 MFL set by US-EPA (Mager et al., 2022). Cement mortar is a significant short-term source of inorganic contamination due to rapid dissolution of constituents upon contact with water (Liu et al., 2022; Młyńska et al., 2019): batch tests showed relevant releases of chromium and lead (10 µg/L and 17 µg/L) within the first 20 days, followed by a consistent decrease (2 µg/L) (Zielina et al., 2022).

Polymeric materials used in DWDN include a wide range of materials, including PVC, HDPE, PP, PE, PEX, PP and PB (Langenbach et al., 2026; Stefan et al., 2023). These materials proved to release in water organic substances (Cheng et al., 2016; Kalweit et al., 2019; Ryssel et al., 2015; M. Shaikh et al., 2019; M. M. Shaikh et al., 2019). For HDPE, 2,4-DTBP is a major migrant (Stefan et al., 2023). Moreover, chemicals related to antioxidants, esters, aldehydes, ketones, terpenoids and aromatic compounds were also identified as leachates (Skjevraak et al., 2003). PEX frequently releases MTBE/ETBE, aldehydes, ketones, alcohols, carboxylic acids, and compounds such as 2,6-di-tert-butyl-p-benzoquinone, 3,5-di-tert-butyl-4-hydroxybenzaldehyde (Kalweit et al., 2019; Ryssel et al., 2015; Stefan et al., 2023). PEX field/lab studies reported individual organics up to 8.0 µg/L and total released non-volatile organic compounds around 0.42 mg/L (Ryssel et al., 2015). PVC generally exhibits lower release under controlled conditions, but it can leach endocrine-disrupting compounds such as nonylphenol (NP) and bisphenol A (e.g., 64-195 ng/L NP in household tap water) as well as volatile organic compounds (VOCs), including chloroform, carbon tetrachloride, and dichloropropane (Cheng et al., 2016; M. Shaikh et al., 2019). Leaching is strongly influenced by temperature, stagnation time, pipe aging, and disinfectants. Residual disinfectants accelerate polymer degradation and significantly increase organic release, including plasticizers and antioxidants (He et al., 2023). These leachates act as DBP precursors: it was found that water disinfected with NaOCl, after being in contact with polymeric pipes, led to the formation of chloroform up to 106 µg/L (Langenbach et al., 2026). Lastly, polymeric materials are also used for the fabrication of gaskets and seals. Studies reported that even these components may be a potential source of organic carbon (Langenbach et al., 2026) and of nitrosamines (Morran et al., 2011; Teefy et al., 2014).

Epoxy resins are used for relining and contain bisphenol A (BPA), epichlorohydrin and polyamines (Cantoni et al., 2021; Pahari et al., 2025). Experiments on relined lead and copper pipes identified BADGE as the main leachate (Lane et al., 2015). New epoxy materials for cured-in-place pipes also contain numerous residual organic compounds: one study found volatile organic compounds (VOCs) and reported leaching of BPA, BADGE (BPA-diglycidylether) and 2-EHGE (2-ethylhexyl glycidyl ether) into drinking water (Pahari et al., 2025). In epoxy-lined household pipes, BPA was detected in most samples, with maxima in cold water of 0.25 µg/L for older lining technology and 10 ng/L for newer one (Rajasärkkä et al., 2016). Some studies also report bisphenol F (BPF) as a substance released by epoxy resins (Bruchet et al., 2014). The presence of disinfectants can result in the formation of DBPs. BPA can indeed react with chlorine-based disinfectants resulting in the formation of chlorophenols, as reported in several studies (Bruchet et al., 2014; Kosaka et al., 2012). Lastly, since polyamines can be used as hardeners in epoxy resins, nitrosamines could be another potential DBP produced from the leachate



of these materials. Amine-containing polymers may indeed act as precursors of nitrosamines, especially when chloramination is performed (Krasner et al., 2013).

A summary of the information gathered from the literature review is provided in Table 3-1.

Table 3-1: Summary of literature review about chemicals leached from materials in contact with water and DBPs formation.

Materials in contact with water	Substances leached	Disinfectant effect
Metals (lead, copper, iron, steel)	- Lead from corrosion scales and solder (up to 9.62 mg/L) - Copper corrosion products (e.g., malachite) - Fe²⁺/Fe³⁺ causing colored water - Other metals from scales: Al, Mn, Ca, Zn	- Chlorine (HOCl/NaOCl) enhances corrosion - Formation of higher oxidation states of metals - Promotes metal release from scales - Biofilm–chlorine interactions → formation of N-DBPs
Cement-based materials (asbestos-cement, cement mortar lining, etc.)	- Major ions: Ca, Si, Al - Trace metals: Cr, Pb, Cd - Asbestos fibers	- Chlorine enhances dissolution/leaching of Ca, Al, Cr, Pb - Alters pH and alkalinity - No strong direct DBP precursor role, but indirect effects via water chemistry changes
Polymers (PVC, PE, PEX, PP, PB, HDPE, etc.)	- Phenols (e.g., 2,4-di-tert-butylphenol (2,4-DTBP)) - Aldehydes, ketones, alcohols, carboxylic acids - Ethers (MTBE/ETBE) - Aromatics (BTEXs) - non-volatile organic compounds - BPA, NP	- Residual disinfectants (Cl₂, ClO₂, O₃) accelerate polymer degradation - Increase DOC (Dissolved Organic Carbon) release (precursors) - Formation of trihalomethanes (THMs) (e.g., chloroform up to about 100 µg/L) - Possible formation of N-nitrosamines (from elastomers/seals)
Epoxy resins	- Bisphenols: BPA and BPF - Ethers: BADGE, 2-EHGE - Additives and VOCs	- Chlorine reacts with BPA leading to the formation of chlorophenols (e.g., 2,4,6-TCP) - Disinfectants accelerate resin degradation and leaching



3.2. Monitoring campaign of newly installed epoxy resins in CS#2

3.2.1. Design of the Campaign

In the CS#2 (Milan) the Comasina DWTP was temporarily stopped to reline a portion of the pipe connecting the outlet of the disinfection reactor to the Point-of-Entry of the DWDN. The DWTP is fed by groundwater, treated by adsorption on granular activated carbon (GAC) followed by disinfection with sodium hypochlorite.

Once the relining was completed, before restarting the DWTP operation, the relined pipe was washed three times using water supplied by a hydrant next to the Comasina DWTP spiked with NaOCl at high concentration. Washing water was discharged into the sewer system. Samples before (point A, see Figure 3-1) and after (point D in Figure 3-1) the relined pipe was monitored as summarized in Table 3-2. Then, the DWTP restarted routine operation and from December 2024 to June 2025 water samples were collected before (point C in Figure 3-1) and after (point D) the relined pipe and in two supply points (points E and F, see Figure 3-1) in the DWDN, at different distances from the DWTP.

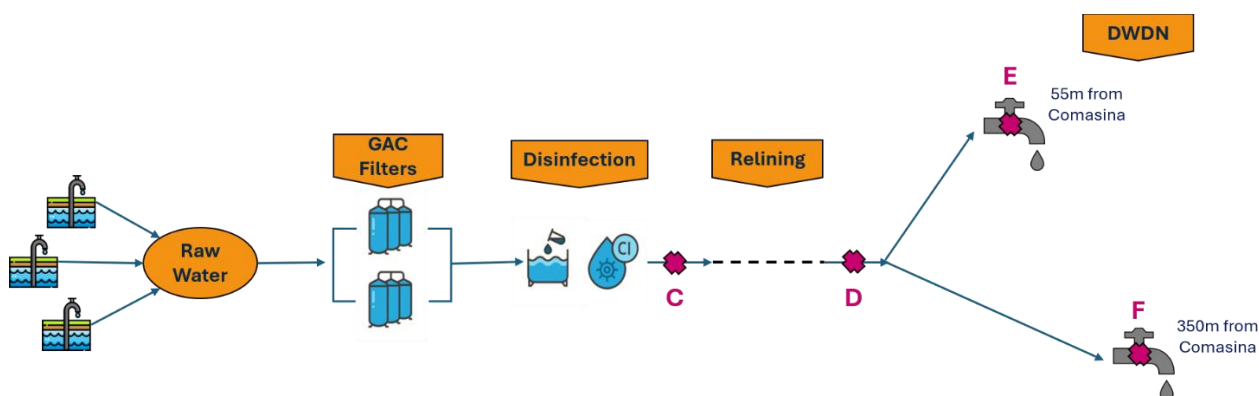


Figure 3-1: Monitoring scheme of the Comasina DWTP during routine operation

Based on the literature review summarized in Chapter 2, a set of parameters was selected, as reported in Table 3-2: bisphenols, amines, chlorophenols, epichlorohydrin and nitrosamines were monitored. BADGE, 2-EHGE and chloro-bisphenols were not monitored due to analytical limitations. Moreover, water macro-parameters (temperature, pH), TOC, absorbance and fluorescence were also monitored, as well as total halogenated organic compounds (TOX), polar DBPs and toxicity. Data below the Limit of Quantification (LOQ) or the Limit of Detection (LOD) were imputed with using half of the LOQ or LOD for all the parameters but toxicity.



Table 3-2: List of monitored parameters during washing and routine operation of Comasina DWTP, and number of samples collected. Washing phase: one sampling for each out of the three washing cycles. Routine monitoring: monthly samples from December 2024 to June 2025.

Parameter	LOQ	Analyzed samples per sampling point	
		Washing	Routine
Macro-parameters	-	3	7
TOC	0.1 mg _C /L		
Absorbance and fluorescence	-	3	7
TOX ⁱ	0.2 µg/L 0.15 µg/L for vinyl chloride	3	7
Polar DBPs	0.02 µg/L for Cl ₂ MSA (LOD) 0.01 µg/L for Br ₂ MSA (LOD)	3	6
Bisphenols ⁱⁱ	2 µg/L 0.75 µg/L for BPA	3	3
Aromatic ⁱⁱⁱ and aliphatic ^{iv} amines	2 µg/L		
Chlorophenols ^v	0.02 µg/L		
Epichlorohydrin	0.05 µg/L		
Nitrosamines ^{vi}	5 ng/L 10 ng/L for NDBA	3	7
Toxicity	Variable with sample size	3	6

ⁱ 1,2-dichloroethane; 1,2-dichloropropane; cis-1,2-dichloroethylene; vinyl chloride; cfc11; cfc113; hcfc141b; methylchloroform; tetrachloromethane; chloroform; bromodichloromethane; dibromochloromethane; bromoform; trichloroethylene; tetrachloroethylene.

ⁱⁱ BPA; bisphenol AF; bisphenol AP; bisphenol B; bisphenol BP; bisphenol C; bisphenol E; BPF; bisphenol FL; bisphenol G; bisphenol M; bisphenol P; bisphenol PH; bisphenol S; bisphenol Z.

ⁱⁱⁱ 2,4-Dimethylaniline; o-Aminoazotoluene; o-Anisidine; o-Toluidine; p-Aminoazobenzene; 1,3-Phenylenediamine; 2,4,5-Trimethylaniline; 2-Naphthylamine; 3,3'-Dichlorobenzidine; 3,3'-Dimethylbenzidine; 3,3'-Dimethoxybenzidine; 4,4'-Diaminodiphenylmethane; 4,4'-Methylenebis(2-chloroaniline); 4,4'-Methylenedi-o-toluidine; 4,4'-Oxydianiline; 4,4'-Thiodianiline; 4-Chloro-o-toluidine; 4-Chloroaniline; 4-Methyl-m-phenylenediamine; 4-Methoxy-m-phenylenediamine; 5-Nitro-o-toluidine; Aniline; Benzidine.

^{iv} Diethanolamine; Diethylamine; Diisopropylamine; Dimethylamine; Dimethylformamide; Ethanolamine; Ethylenediamine; Tributylamine; Triethanolamine; Triethylamine.

^v 2,4,6-Trichlorophenol; 2,4-Dichlorophenol; Pentachlorophenol; 2-Chlorophenol.

^{vi} N-Nitrosodi-n-propylamine; N-Nitrosodi-n-butylamine (NDBA); N-Nitrosodiethylamine; N-Nitrosodimethylamine (NDMA); N-Nitrosomethylethylamine; N-Nitrosomorpholine (NMOR); N-Nitrosopiperidine; N-Nitrosopyrrolidine.



3.2.2. Analytical methods

The analytical method for the analysis of aliphatic amines is the following. The (aqueous) samples were filtered and analyzed directly by liquid chromatography coupled with a triple quadrupole detector. The chromatographic column used is equipped with an octadecyl (C18) stationary phase modified to improve the separation of this class of compounds, while ionization occurs via an Electrospray (ESI) source. Separation is achieved using a binary linear gradient of water/acetonitrile, with ammonium acetate and formic acid. Concerning aromatic amines, the water samples were also filtered and directly analyzed through liquid chromatography coupled with a triple quadrupole detector. The chromatographic column was the same used for aliphatic amines, ionization was performed through ESI source. The separation is obtained using a binary linear gradient water/acetonitrile, with only formic acid.

Concerning epichlorohydrin, it was measured following the EPA procedure EPA 5030C 2003 + EPA 8260D 2018 (Environmental Protection Agency, 2003, 2018a). Chlorophenols were analyzed following the EPA 3510C 1996 + EPA 8270E 2018 (Environmental Protection Agency, 1996, 2018b).

Regarding the analysis of bisphenols, the water sample was filtered and analyzed directly by liquid chromatography coupled with a triple quadrupole detector. The chromatographic column employed is equipped with a biphenyl stationary phase, which ensures high selectivity for this class of compounds, while ionization is carried out via an ESI source. Separation is achieved using a binary linear gradient of water/methanol, without modifiers.

Concerning nitrosamines, water samples were adsorbed onto EnviCarb-type activated carbon solid phase extraction (SPE) cartridges, previously conditioned, to retain the analytes of interest. Subsequently, the analytes were eluted from the cartridge with dichloromethane. A solvent exchange was then carried out to make it compatible with the injection phase: the dichloromethane was evaporated and the residue was reconstituted with ultrapure water. In this case as well, the analysis was performed by liquid chromatography coupled with a triple quadrupole detector, with ionization via an atmospheric pressure APCI source. Chromatographic separation was achieved using a column with an octadecyl (C18) stationary phase, employing a binary linear gradient of water/methanol acidified with formic acid.

The other parameters were analysed following the same procedure as illustrated in Deliverable 2.5.

Regarding toxicity, two types of samples were analysed during each sampling day: water samples and a blank control. The calculation of the toxicity had to be done subtracting the blank to the toxicity of the water sample. However, both the water samples and the blank controls had variable LOQ, depending on factors such as the volume of the water sample. Hence, the imputation of the data was done following this pipeline:

- Water sample toxicity data were fitted calculating the posterior in a model with log-Student-t likelihood and vague prior, using the proper cumulative distribution function for censored data.
- Censored data were imputed using the a posteriori expected value. For data above the LOQ, the observed value was reported.
- Perform previous two points also for blank controls.
- Calculate the difference between water samples data and blank controls. This difference is the actual toxicity of the water sample.
- If the difference is lower than 0, set it to 0.



3.2.3. Results from the washing of relined pipe

The monitoring of the washing step permitted the assessment of immediate leaching of chemicals from the pipe. Moreover, since chlorination was done, even the formation of DBPs could be assessed. The concentration of bisphenols, aromatic and aliphatic amines, epichlorohydrin and chlorophenols were below the LOQ. Concerning nitrosamines, only NMOR was detected. Concentration data are reported in Figure 3-2. The reduction of the concentration of NMOR over the different washing steps suggests that it was an effective cleaning solution for the relined pipes. Moreover, the presence of the compound even at the inlet of the relining may be an indicator of some background contamination.

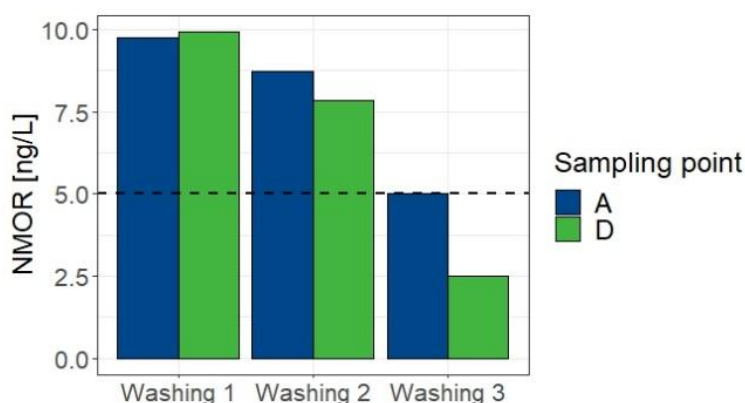


Figure 3-2: NMOR concentration before and after the relining during washing steps. The horizontal dashed line represents the LOQ of 5 ng/L. Sampling points A and D are located before and after the relined pipe

Organic matter was evaluated through different parameters, as illustrated in Figure 3-3. Starting from UVA254, the values were generally low and it was difficult to distinguish between actual differences and the noise of the instrument. Integral fluorescence did not decrease over the washing steps. However, values after the relined pipes were always lower compared to the inlet, suggesting that potentially released organic compounds are not fluorescent. The TOC, differently from integral fluorescence, shows an increase after the relining, especially after the second washing, where a peak of over 2 mgC/L was measured.

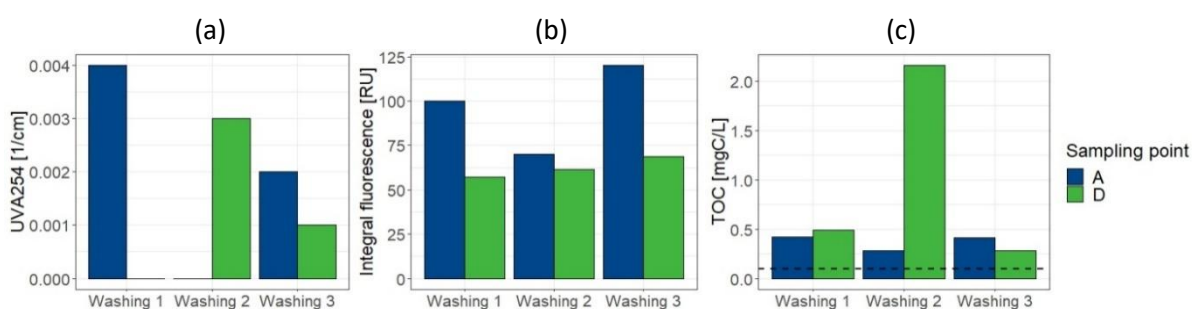


Figure 3-3: Organic matter concentration over washing steps: (a) UVA254; (b) Integral fluorescence; (c) TOC, where the horizontal dashed line represents the LOQ of 0.1 mgC/L. Sampling points A and D are located before and after the relined pipe



The TOX and total trihalomethanes (TTHMs) concentration over the three washing steps are shown in Figure 3-4. Consistently with TOC, TOX and TTHMs concentration increased consistently in water samples from the first two washings, exceeding 600 µg/L in the second one, being chloroform the most present in water samples. Such an increase could have been caused by leaching of organic substances, acting as precursors of DBP formation, also enhanced by intense chlorination.

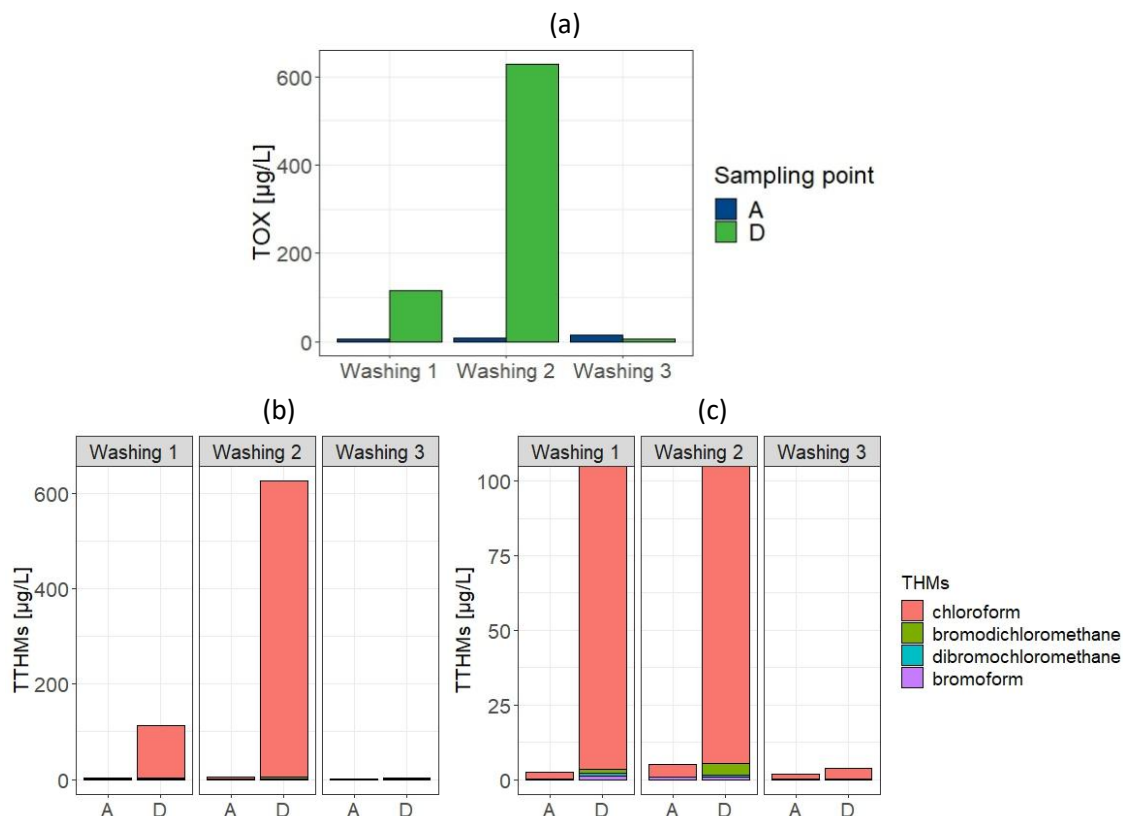


Figure 3-4: TOX (a) and TTHMs (b, c) concentration over the washing steps. In chart c the y-axis range was reduced to 0-100 µg/L for a better visualization. Sampling points A and D are located before and after the relined pipe.

Polar DBPs were also monitored and provided useful information to assess and confirm the effectiveness of the washing procedure. The results are shown in Figure 3-5. In the first two washings, Cl₂MSA concentration increased consistently with THMs, TOX and TOC data. Differently, Br₂MSA concentration decreased during the second washing, potentially due to different precursors between brominated polar DBPs and chlorinated ones. In Figure 3-5c the semi-quantitative data, expressed in peak intensity, is reported for a wider set of polar DBPs: a significant formation of polar DBPs were observed during the first two washings.



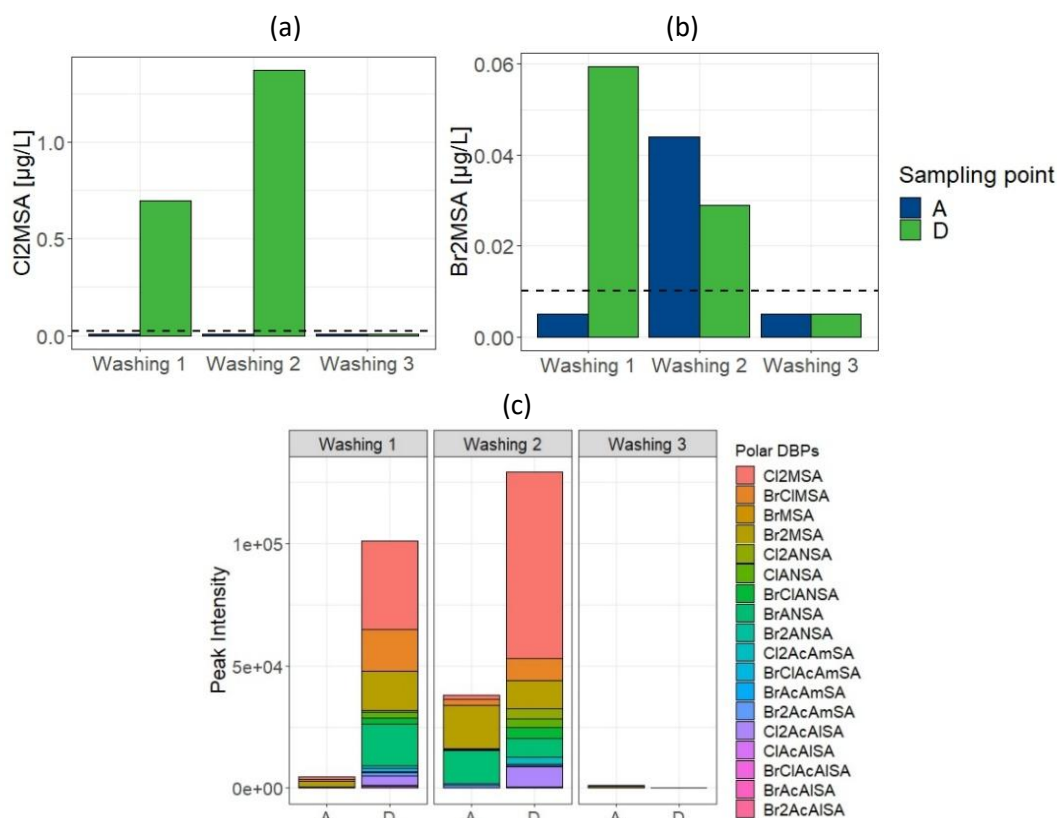


Figure 3-5: Polar DBPs concentration over the washing steps: (a) quantitative data of Cl₂MSA, where the horizontal dashed line is the LOD of 0.02 µg/L; (b) quantitative data of Br₂MSA, where the horizontal dashed line is the LOD of 0.01 µg/L; (c) semi-quantitative data (peak intensity) of a wider set of polar DBPs. Sampling points A and D are located before and after the relined pipe.

Regarding toxicity, results are reported in Figure 3-6. Results about cytotoxicity, ERa and P53 were always below the LOQ. Anti_AR and TTR-TRb toxicity data were generally low. Nrf2, PAH and PXR frequently exceeded the effect-based threshold (EBT) value in washing water.

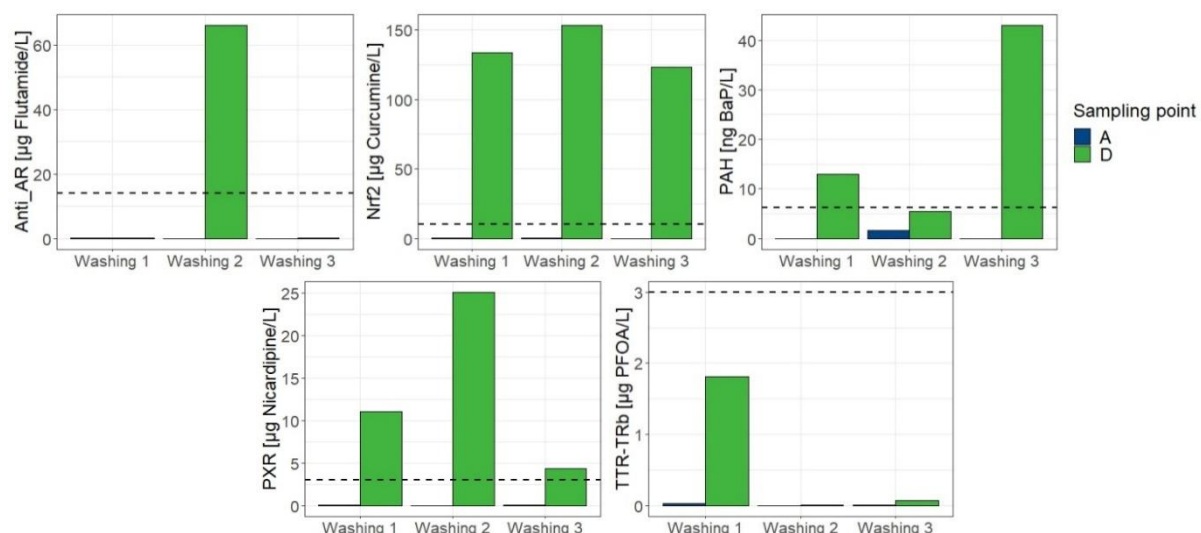


Figure 3-6: Results of toxicity assays over the washing steps. Sampling points A and D are located before and after the relined pipe. The horizontal dashed line represents the EBT values: 14 µg Flutamide/L for Anti_AR, 10 µg Curcumin/L for Nrf2, 6.2 ng BaP/L for PAH, 3 µg Nicardipine/L for PXR and 3 µg PFOA/L for TTR-TRb.



3.2.4. Results from the routine DWTP operation after relining

Bisphenols, aromatic and aliphatic amines, epichlorohydrin and chlorophenols were always below the LOQ. Nitrosamines were the only detected class of compounds. In detail, NMOR and NDMA were detected as shown in Figure 3-7. NMOR was frequently detected in all the sampling points, and its concentration increased over the 100 days of monitoring. NDMA was quantified only in 2 out of 7 samples per sampling point during the first and half months. Boxplots in Figure 3-7c consider only data above LOQ, hence they do not represent the actual NDMA distribution over the entire monitoring period.

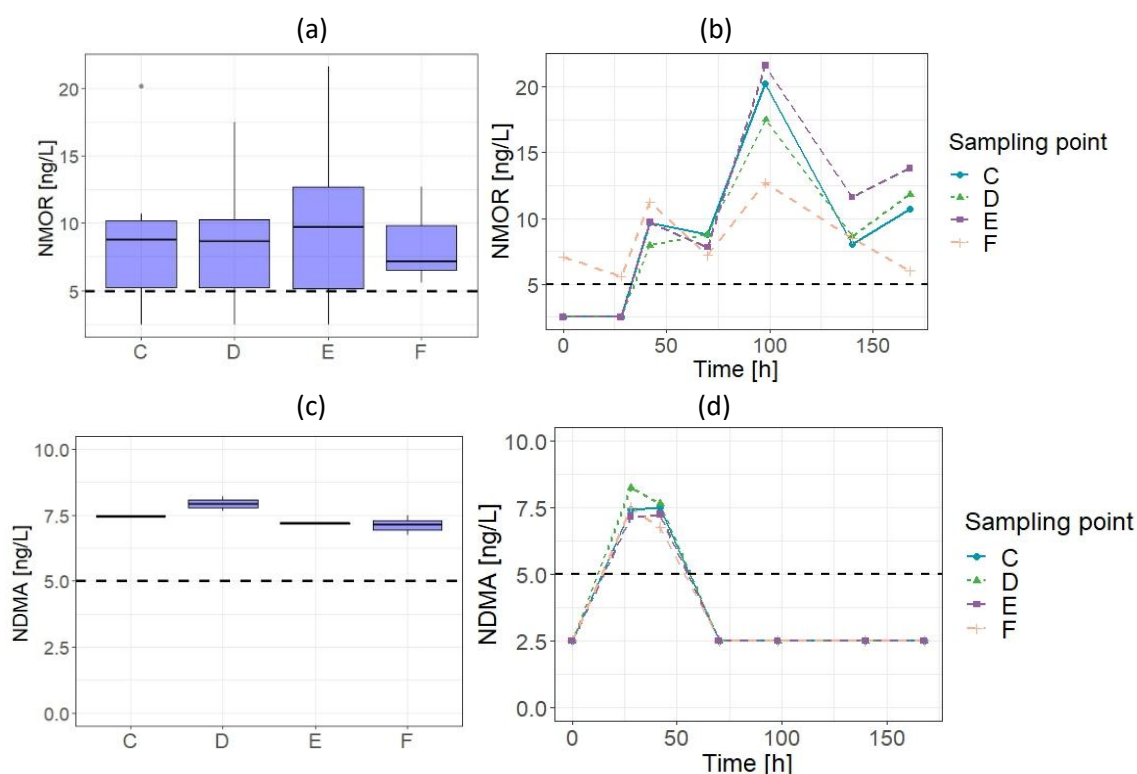


Figure 3-7: Concentration of NMOR (a, b) and NDMA (c, d) during routine DWTP operation: (a, c) distribution over the sampling points ($n=7$); (b, d) time-trend per sampling point. The horizontal dashed line represents the LOQ of 5 ng/L. Box plots for NDMA consider only data over the LOQ.

Concerning organic matter, results are shown in Figure 3-8. UVA254 distribution was stable over the network, displaying higher values than those found during washings. The time trend highlights an increase in this parameter overtime, especially in sampling points D and E. Differently, integral fluorescence and TOC display an increasing trend over the network, especially in sampling point F, which is further from the DWTP compared to sampling point E. In agreement with UVA254 data, both integral fluorescence and TOC displayed an increasing trend during the last two monitoring months, except for sampling point F.



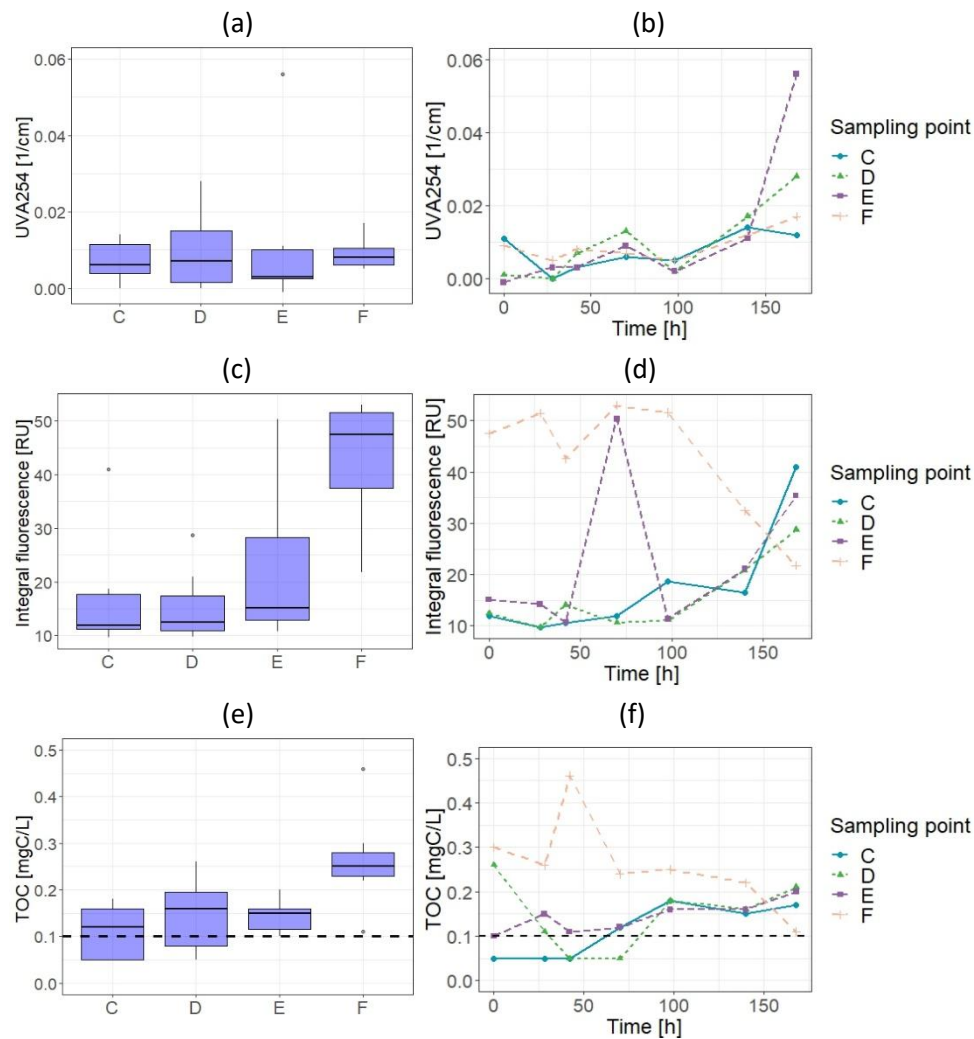


Figure 3-8: Organic matter distribution ($n=7$) (a, c, e) and time-trends (b, d, f) of UVA254 (a, b), Integral fluorescence (c, d) and TOC (e, f) during routine DWTP operation. The horizontal dashed line in the TOC graphs represents the LOQ of 0.1 mgC/L.

The distribution and time-trend of TOX over the sampling points is shown in Figure 3-9. A slow but constant increase in all the sampling points but the F after the first two months can be observed. The composition of TOX is shown in Figure 3-9c. The peak in sampling points C and D after nearly 50 days of monitoring is mainly caused by an anomalous increase of tetrachloroethylene. On the other hand, the slow but constant increase of TOX that occurs after the first two months of sampling seems to be mainly caused by chloroform.



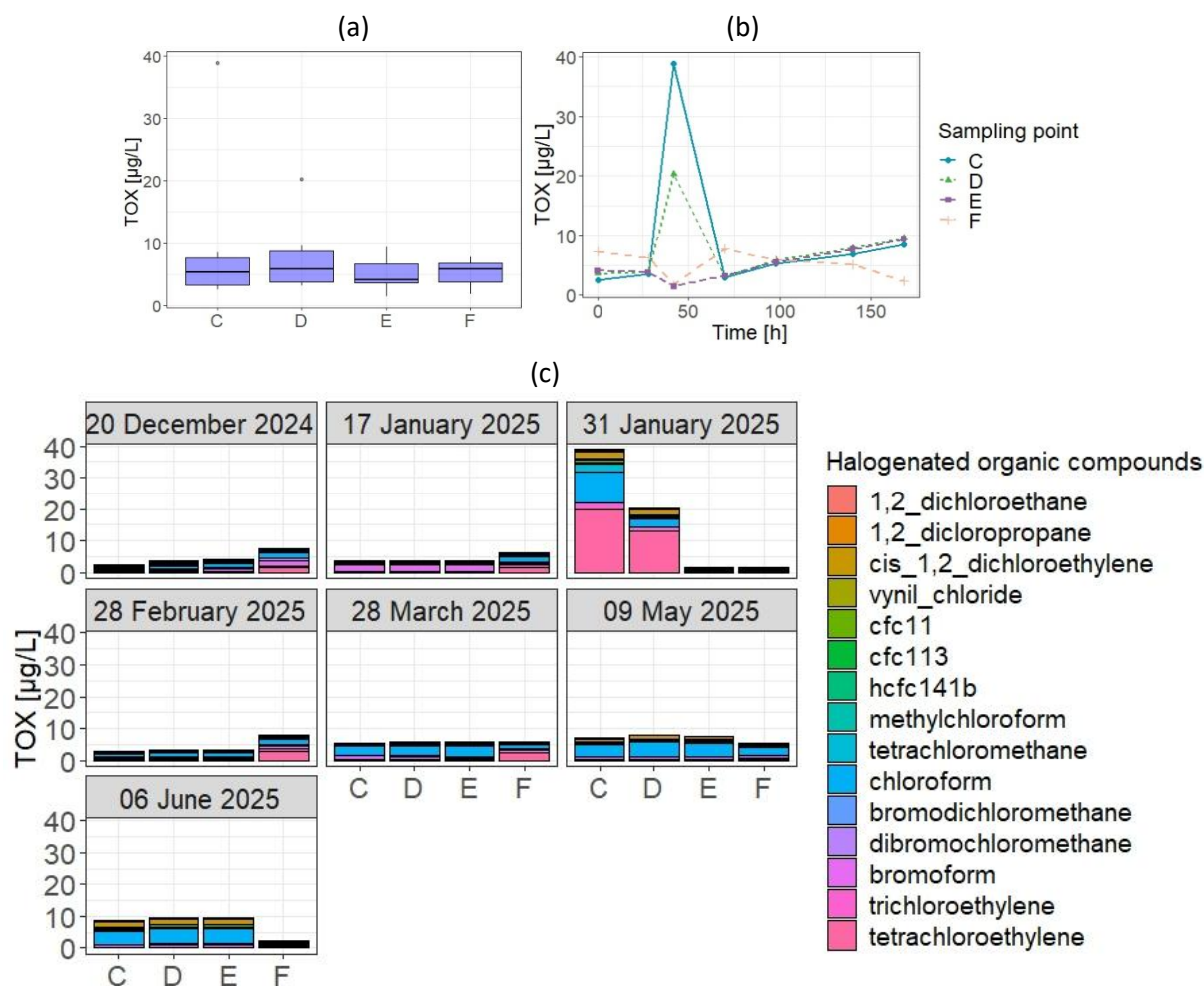


Figure 3-9: TOX data during routine monitoring campaign: (a) distribution over sampling points ($n=7$); (b) time-trends; (c) TOX composition over sampling points.

Concerning polar DBPs, quantitative data are reported for Br2MSA in Figure 3-10, since Cl2MSA was always below the LOD. Br2MSA is formed right after disinfection and decreased over the network. Analyzing the time trend in each sampling point, after the first two months in which concentrations were close or below the LOQ, an increase was observed in all the sampling points but F. This is in agreement with the presence of polar DBPs over the network: while in the first three sampling days the presence of polar DBPs seems to be more in sampling point F compared to the others, the trend switched in the second half of the monitoring campaign.



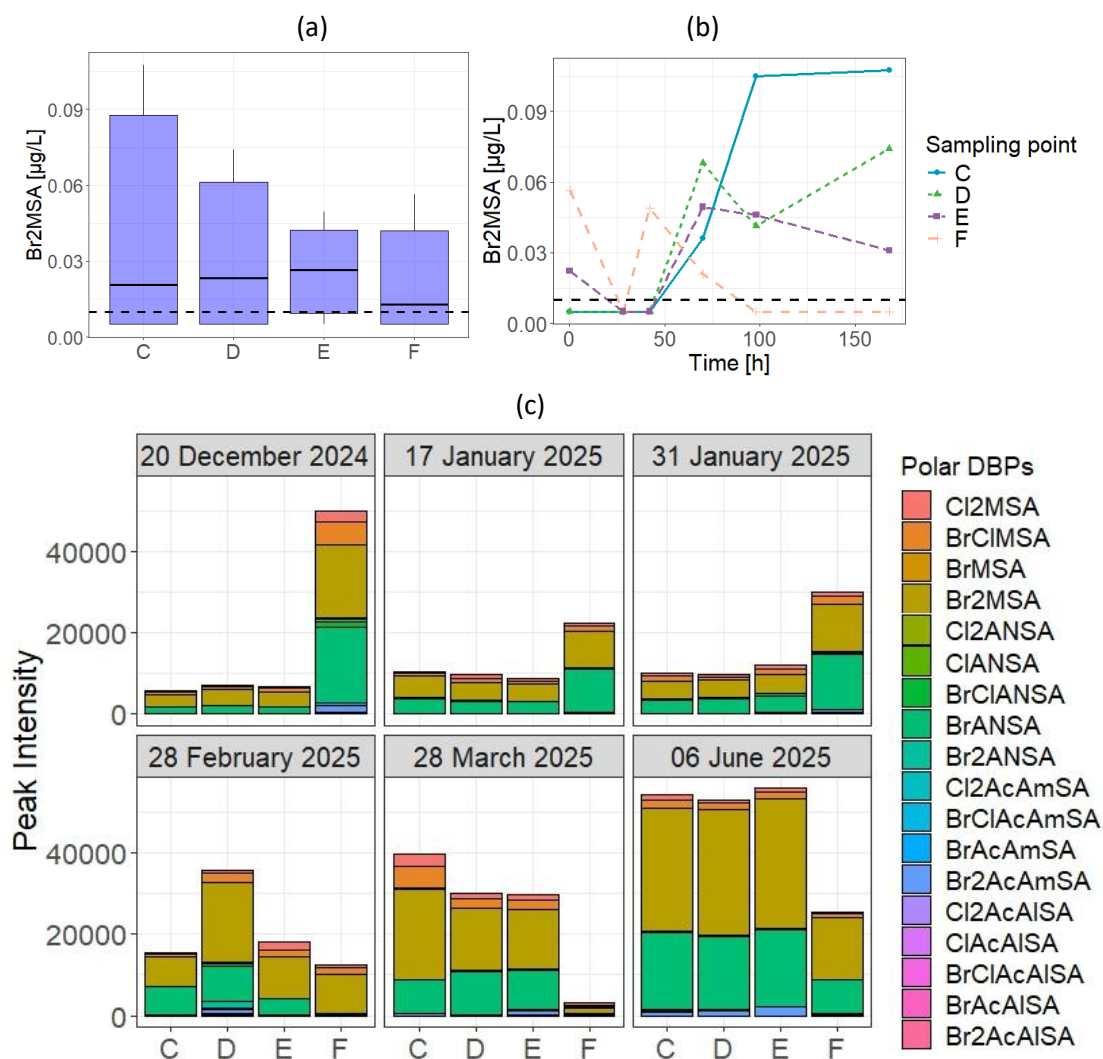


Figure 3-10: Polar DBPs concentration during routine DWTP operation: (a) Br₂MSA distribution over sampling points (n=6) and (b) time-trends; (c) semi-quantitative data of polar DBPs over the network.

Toxicity data are shown in Figure 3-11. The only types of toxicity detected were PAH, PXR and TTR-TRb, while the other ones were below the LOQ. Starting from PAH, it was the most frequently detected toxicity and with the highest number of samples above the EBT. Interestingly, this parameter showed an increase during the last two sampling dates, as done by TOX, Br₂MSA and parameters related to organic matter. Even if this type of toxicity is mostly related to PAH, BaP being the reference compound, also other substances might produce the same type of activity, contributing to its variations.



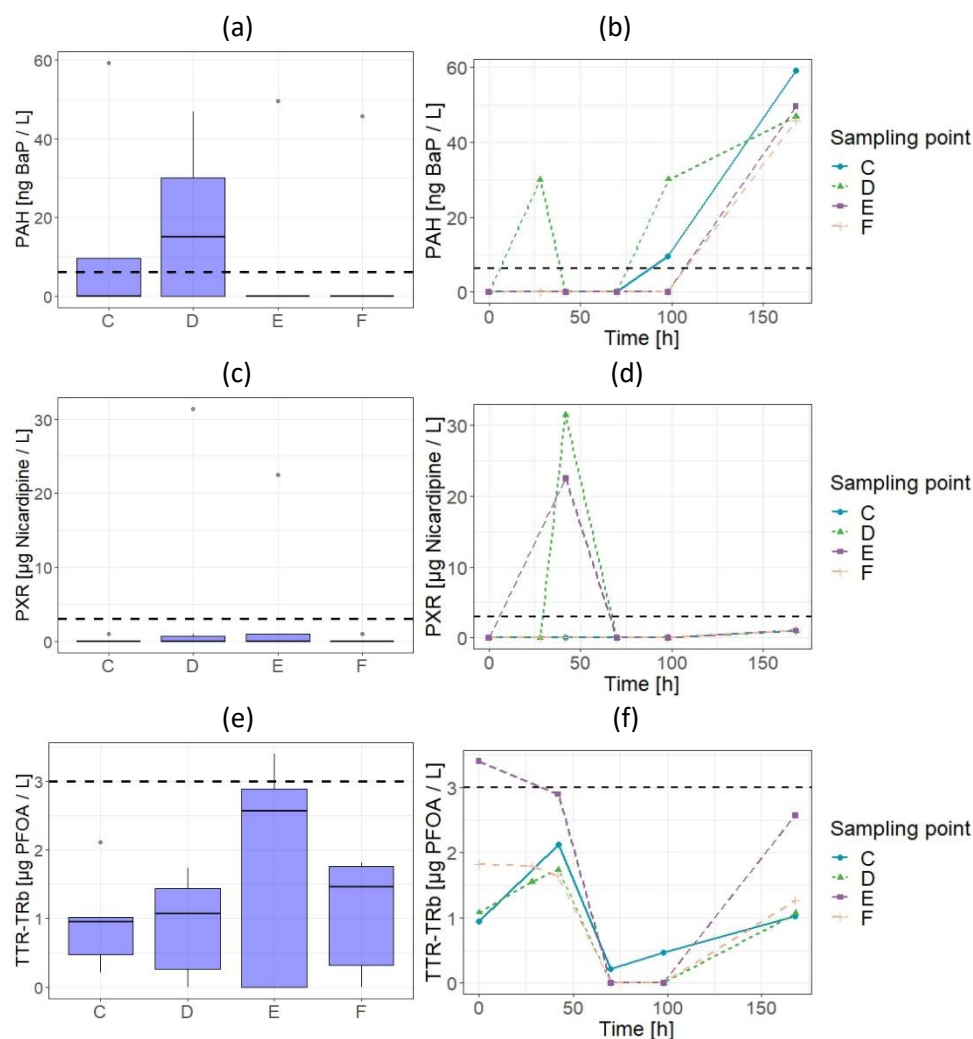


Figure 3-11: Distribution (n=6) (a, c, e) and time-trends (b, d, f) over sampling points of PAH (a, b), PXR (c, d) and TTR-TRb (e, f) activities during the routine DWTP operation. The horizontal dashed line represents the EBT values: 6.2 ng BaP/L for PAH, 3 µg Nicardipine /L for PXR and 3 µg PFOA /L for TTR-TRb.

3.3. Experimental evaluation of the uptake of contaminants leaching from materials

Results obtained from the literature review (Chapter 3.1) and the monitoring campaign (Chapter 3.2) were used to support the design of experimental activities aimed at assessing the uptake of contaminants leached from materials in contact with water in sprouts, used as reference for home-grown vegetables.

3.3.1. Experimental plan and set-up

The literature review (Chapter 3.1) identified bisphenols, mainly BPA and BPF, as relevant chemicals released into water. Moreover, the monitoring campaign in CS#2 (Chapter 3.2) confirmed the presence of two nitrosamines, NDMA and NMOR, in drinking water. For this reason, BPA, BPF, NDMA and NMOR were selected as reference compounds. The concentration ranges were set based on both literature data and outputs of the monitoring campaign and reported in Table 3-3.

Uptake and phytotoxicity experiments were performed using two sprouts: alfalfa (*Medicago sativa*) and radish (*Raphanus sativus*). The experimental plan was designed using the Design of Experiments



(DoE) methodology and organized in two steps: screening and optimization. The screening step was performed based on a Full Factorial Design, exploring all the possible combinations between the extremes of the levels (concentration values in Table 3-3) of the four contaminants. The screening led to the selection of the two most significant chemicals, which were then investigated in the optimization step performed based on a Central Composite Inscribed design, according to the Response Surface Methodology.

Table 3-3: Experimental plan according to DoE.

Step	BPA [$\mu\text{g/L}$]	BPF [$\mu\text{g/L}$]	NDMA [ng/L]	NMOR [ng/L]
Screening	24.75	31.65	9.72	13.20
	24.75	31.65	9.72	7.73
	24.75	31.65	1.62	13.20
	24.75	31.65	1.62	7.73
	24.75	5.28	9.72	13.20
	24.75	5.28	9.72	7.73
	24.75	5.28	1.62	13.20
	24.75	5.28	1.62	7.73
	4.13	31.65	9.72	13.20
	4.13	31.65	9.72	7.73
	4.13	31.65	1.62	13.20
	4.13	31.65	1.62	7.73
	4.13	5.28	9.72	13.20
	4.13	5.28	9.72	7.73
	4.13	5.28	1.62	13.20
	4.13	5.28	1.62	7.73
Optimization	12.38	0	9.72	7.73
	21.12	0	8.29	7.73
	24.75	0	4.86	7.73
	21.12	0	1.62	7.73
	12.38	0	0	7.73
	3.62	0	1.62	7.73
	0	0	4.86	7.73
	3.62	0	8.29	7.73
	12.38	0	4.86	7.73



For BPA, BPF and NDMA, analytical standards were purchased from Sigma Aldrich. Stock solutions were prepared in deionized water, having concentrations respectively equal to 1.65 mg/L, 2.11 mg/L and 5.40 µg/L. Concerning NMOR, two samples of drinking water were collected and used as stock solution, having 13.20 ng/L and 7.73 ng/L respectively.

For the experiments, the stock solutions of NMOR were spiked with those of BPA, BPF and NDMA and 5 mL were poured in a petri dish where a filter paper was placed supporting 10 seeds of alfalfa or radish. For each experiment, corresponding to a row in Table 3-3, six replicates were performed, i.e. six petri dishes. The dishes were stored at 22.5°C, with a photoperiod of 12 h for 7 days and providing full-spectrum LED illumination. After 5 days of incubation, 5 mL of sample were spiked again to prevent the water from drying out completely. Control experiments were also performed following the same procedure without spiking contaminants.

After incubation, the germinated seeds (sprouts) were pooled and frozen at -20°C overnight. Frozen sprouts were fragmented manually using sterile scalpels and the homogenized biomass was weighted and divided into two aliquots of equal mass for extract preparation. Surrogate standards were added to each aliquot at concentrations corresponding to five times the LOQ defined by the external analytical laboratory (Table 3.1). BPA and BPF surrogates were spiked into the aliquot designated for bisphenol extraction, and NDMA surrogate was spiked into the aliquot designated for nitrosamine extraction. NMOR was not spiked. Surrogates added to the control samples were used to assess extraction recovery efficiency. Extract for bisphenol analysis was prepared adding acetonitrile in a 1:1 ratio (1 mL per 1 g of fresh sprouts), vortexing for 5 minutes and then centrifuging for 10 minutes at 3000 rpm; the upper acetonitrile layer was transferred into a glass vial, where n-hexane was added in 1:1 ratio (1 mL per 1 g of fresh sprouts), vortexed for 5 minutes and centrifuged for 10 minutes at 3000 rpm; the upper n-hexane layer was transferred into a 50 mL glass vial and evaporated under a mild nitrogen gas stream; after complete evaporation, the dried residue was resuspended with acetonitrile to a final volume of 50 mL, and sent to the external lab for analysis. Extracts for nitrosamine analysis was prepared adding dichloromethane (DCM) in a 4:1 ratio (4 mL per 1 g of fresh sprouts), placed in a ultrasonic bath for 30 minutes, and then centrifuged for 15 minutes at 3000 rpm; the DCM was collected and evaporated to dryness using a mild nitrogen gas stream; after complete evaporation, the dried residue was resuspended with deionized water to a final volume of 1 L, and sent to the external analytical lab for analysis.

The analytical methods for the analysis of bisphenols and nitrosamines are reported in Chapter 3.2.1.

The calculation of the uptake was done multiplying the concentration of the extract (E) by its volume (V) and dividing by the mass of the extraction aliquot (M_e) expressed in grams of wet weight sprouts (g_{ww}).

$$Uptake = \frac{E * V}{M_e} \quad (3.1)$$

The concentration of the extract was expressed in µg/L for bisphenols and in ng/L for nitrosamines. The volume of the extract was 0.05 L for bisphenols and 1 L for nitrosamines. Hence, for bisphenols the uptake was expressed in µg/ g_{ww} , while for nitrosamines in ng/ g_{ww} .



3.3.2. Results of the germination and uptake experiments

The results of the screening experiments with alfalfa are shown in Figure 3-12. Results of radish were all below LOQ, hence, they are not reported. Alfalfa experiments highlighted how only nitrosamines can be bioaccumulated in the sprouts, especially NMOR, at the tested concentration. Moreover, NDMA showed a potential interaction with bisphenols: NDMA uptake was identified only when BPA was set to the minimum concentration, suggesting that high bisphenols concentrations may reduce the uptake of nitrosamines. Lastly, a decreasing uptake trend can be observed with respect to the germinated mass. Concerning the optimization, both the experiments with alfalfa and radish produced results below LOQ.

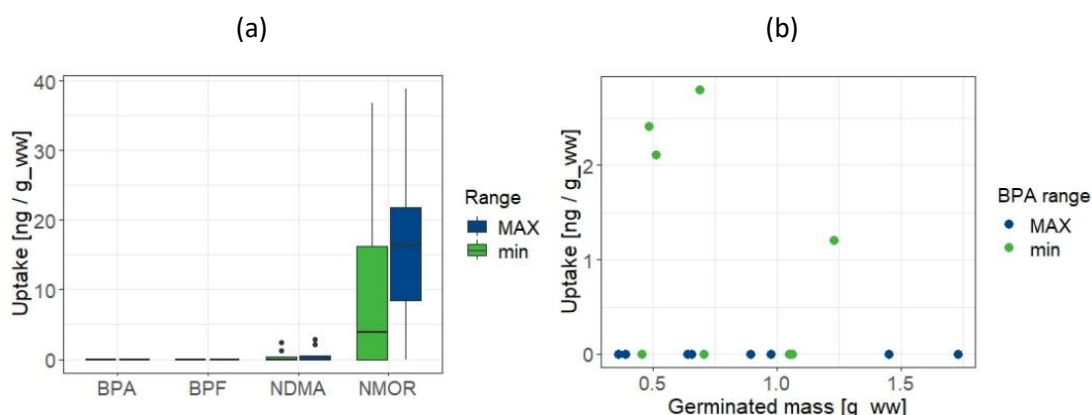


Figure 3-12: Screening results of uptake of contaminants on alfalfa: (a) distribution of uptake results by contaminant and concentration (n=8); (b) interaction between the uptake of NDMA and BPA.

3.4. Human health risk assessment

We developed a human health risk assessment framework to account for the overall ingestion of contaminants leached into drinking water considering as exposure routes drinking water ingestion and consumption of home-grown vegetables. Experiments described in Chapter 3.3 (screening step with alfalfa) were the basis and additional risk scenarios were also considered.

3.4.1. Methodologies

The procedure to calculate the risk was the following: firstly, the average daily dose (ADD) was calculated:

$$ADD = \frac{C \cdot IR}{BW}, \quad (3.2)$$

where C is the concentration of the contaminant, either expressed in $\mu\text{g/L}$ for water or in $\mu\text{g/g}_{\text{ww}}$ for sprouts, IR is the ingestion rate (L/day for water; $\text{g}_{\text{ww}}/\text{day}$ for sprouts). BW is the body weight of the consumer, expressed in kg. Hence, ADD is expressed in $\mu\text{g}/(\text{day} \cdot \text{kg})$.

Table 3-4: Exposure parameters used for different scenarios of risk assessment. P50 and P95 refer to the 50th and 95th percentiles of the lognormal distribution of IR obtained from EFSA statistical data.

Scenario	IR water (L/day)	BW (kg)	IR alfalfa P50 ($\text{g}_{\text{ww}}/\text{day}$)	IR alfalfa P95 ($\text{g}_{\text{ww}}/\text{day}$)	IR radish P50 ($\text{g}_{\text{ww}}/\text{day}$)	IR radish P95 ($\text{g}_{\text{ww}}/\text{day}$)
Omnivore adult	2	70	3.16	31.9	10	10
Omnivore toddler	1	20	2.17	10.02	5.94	12
Vegetarian adult	2	70	10.5	32.8	3.09	8.23



Multiple scenarios have been considered based on consumer age and dietary: omnivore adults and toddlers, and vegetarian adults, whose IR and BW values are summarized in Table 3-4. Regarding IR, two scenarios of exposure were defined assuming a lognormal distribution, based on statistical data provided by EFSA, and calculating the 50th (P50) and the 95th (P95) percentiles.

The ADD from sprouts (ADD_s) and from water (ADD_w) were summed, giving the total ADD (ADD_t). Then, depending on the type of risk, acute for bisphenols and chronic for nitrosamines, the risk was assessed in terms of hazard quotient (HQ) or increased life cancer risk (ILCR):

$$HQ = \frac{ADD_t}{TDI \text{ or } RfD'} \quad (3.3)$$

$$ILCR = ADD_t * SF. \quad (3.4)$$

The TDI is the Tolerable Day Intake ($\mu\text{g}/\text{kg} \cdot \text{day}$) and was used for BPA. For BPF, since a Reference Dose (RfD) was available, it was used to calculate the HQ. SF is the slope factor. The values adopted for these parameters and the sources are summarized in Table 3-5.

Table 3-5: Toxicological reference values used to calculate HQ and ILCR.

Contaminant	Risk type	Toxicological Index	Reference Value	Target	Source
BPA	Acute	TDI [$\text{ng}/(\text{kg} \cdot \text{day})$]	0.2	Immune system	(Lambré et al., 2023)
BPF	Acute	RfD [$\text{ng}/(\text{kg} \cdot \text{day})$]	8.09	Reproductive system	(Cao et al., 2025)
NDMA	Chronic	SF [$(\text{mg}/(\text{kg} \cdot \text{day}))^{-1}$]	51	Liver	(EPA Federal Facilities Restoration & Office, 2014)
NMOR	Chronic	SF [$(\text{mg}/(\text{kg} \cdot \text{day}))^{-1}$]	6.7	Liver	(OEHH - State of California, 2009)

To evaluate how much of the overall risk comes from water and from sprouts respectively, risk apportionment was calculated as:

$$Risk \text{ apportionment}_w(\%) = \frac{Risk_w}{Risk_s + Risk_w} * 100, \quad (3.5)$$

$$Risk \text{ apportionment}_s(\%) = \frac{Risk_s}{Risk_s + Risk_w} * 100. \quad (3.6)$$

where Risk represents HQ or ILCR.

An additional risk scenario was also developed setting the concentration of each contaminant at its LOQ. The risk was calculated as previously explained, but only the P50 IR of sprouts were considered.

3.4.2. Results of the risk assessment

The overall human risk estimated using the experimental results with alfalfa is reported in Figure 3-13, which represents different scenarios. No relevant differences emerge between different dietary habits, and the risks exceed the threshold in all the scenarios considered.

To point out the main risk source, the apportionment of the risk between drinking water and sprout consumption is shown in Figure 3-14. Independently from the age of consumers or their dietary habits, the main source of risk due to NDMA comes from drinking water, while the risk due to NMOR is



comparable for drinking water and sprout consumption. These results derive from experimental evidence since NDMA bioaccumulation is negligible on alfalfa sprout compared to NMOR (Chapter 3.3).

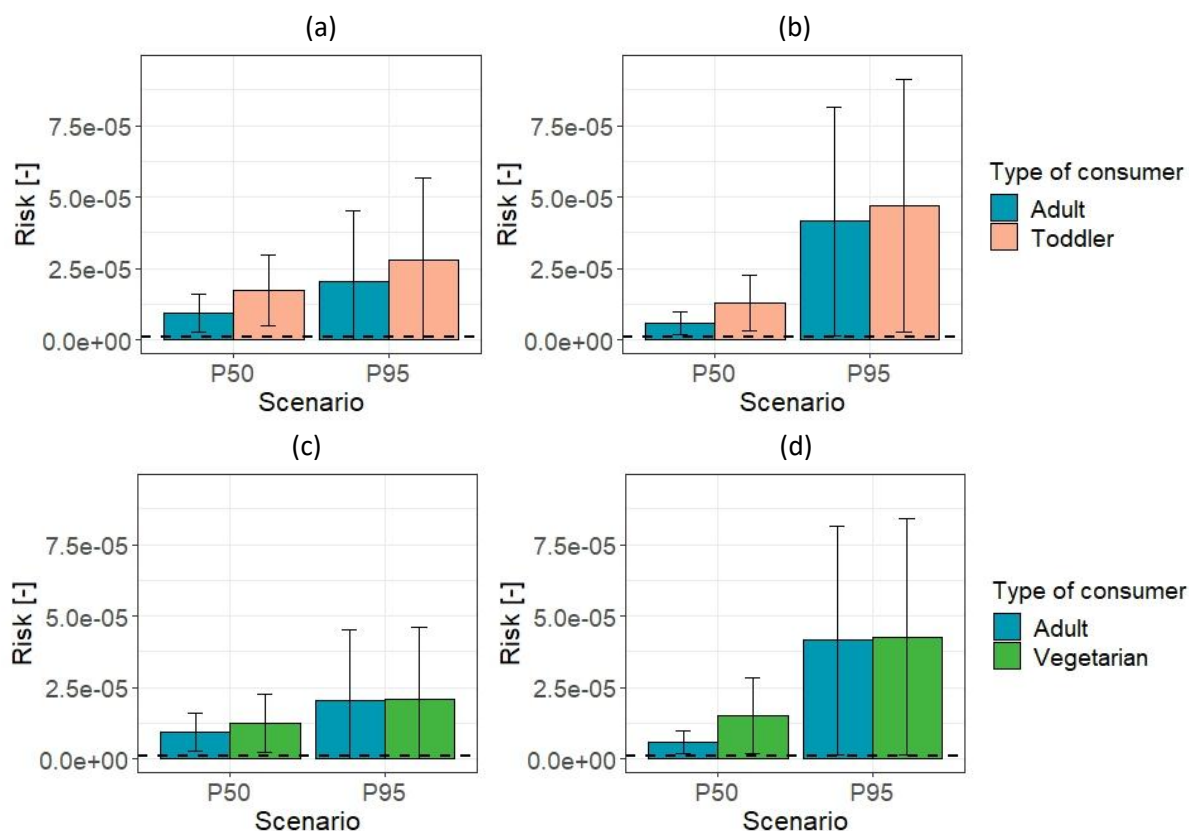


Figure 3-13: Risk results from experimental screening on alfalfa (n=16): NDMA (a,c) and NMOR (b,d). The horizontal dashed line represents the risk threshold of 10^{-6} .

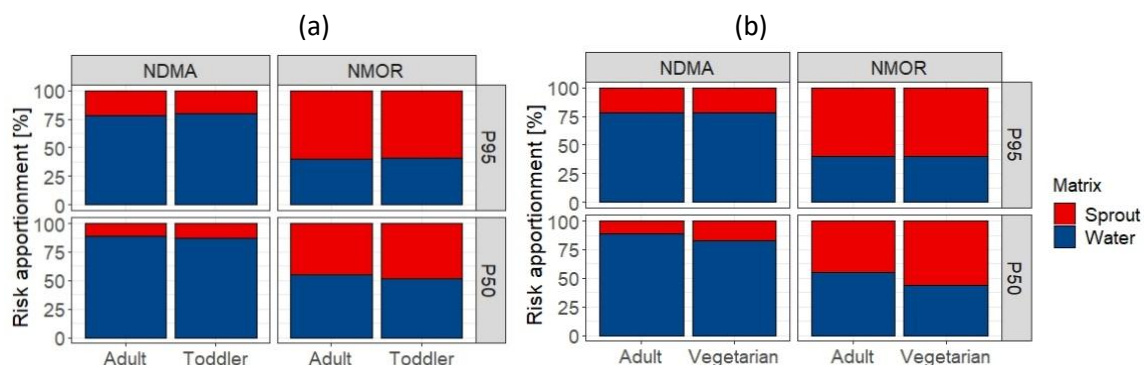


Figure 3-14: Risk apportionment between drinking water consumption and sprout consumption comparing: (a) adults and toddlers; (b) adult dietary habits (data from screening experiments with alfalfa).

Results for the risk scenario in which contaminant concentrations are set equal to their LOQ are reported in Figure 3-15, for both alfalfa and radish sprouts. Interestingly, just setting the concentration to the LOQ results in the exceedance of the risk threshold in every considered situation. Toddlers seem to be the most affected consumer, showing the highest risk values both in terms of HQ, exceeding 200 in the case of BPA, and of ILCR, approaching $4 \cdot 10^{-4}$ with NDMA. This highlights the fact that there is a need to reduce the LOQ values for these pollutants. LOQ should be indeed small enough to detect



situations where the risk is not already too high, to be able to promptly detect dangerous situations that require utility operators to take actions.

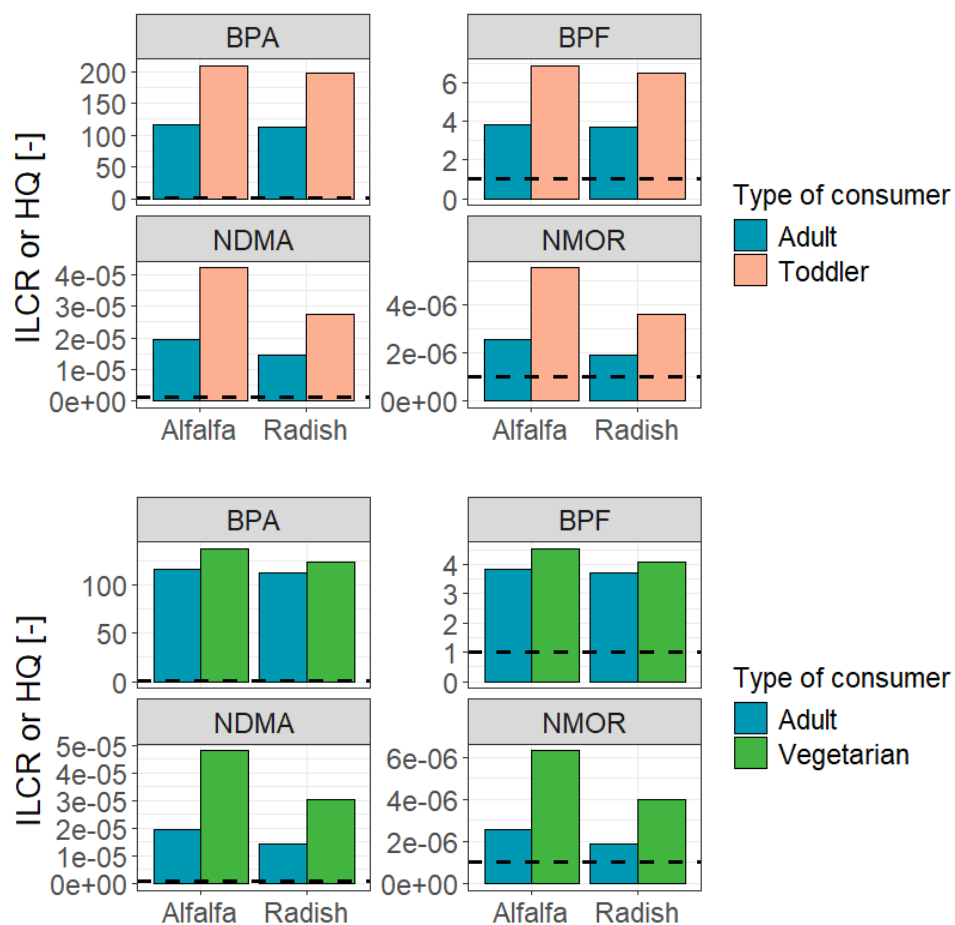


Figure 3-15: Risk estimation when contaminant concentrations are set at their LOQ. The horizontal dashed lines represent the risk threshold, which is set to 1 for bisphenols and to 10^{-6} for nitrosamines.

The assessment of how much water and sprouts contributed to the overall risk in the above considered scenario can be done in Figure 3-16. As was found from experimental data, the apportionment is similar between omnivore adults and toddlers. However, in this case the contribution of sprouts to the overall NDMA risk is higher than before. Concerning bisphenols, on the contrary, risk is mostly coming from water. Moving to the comparison between omnivore and vegetarian adults, the differences are more pronounced. Moreover, risk related to nitrosamines for vegetarians is mainly coming from sprouts. On the other hand, water is even for vegetarians the main source of risk related to bisphenols.



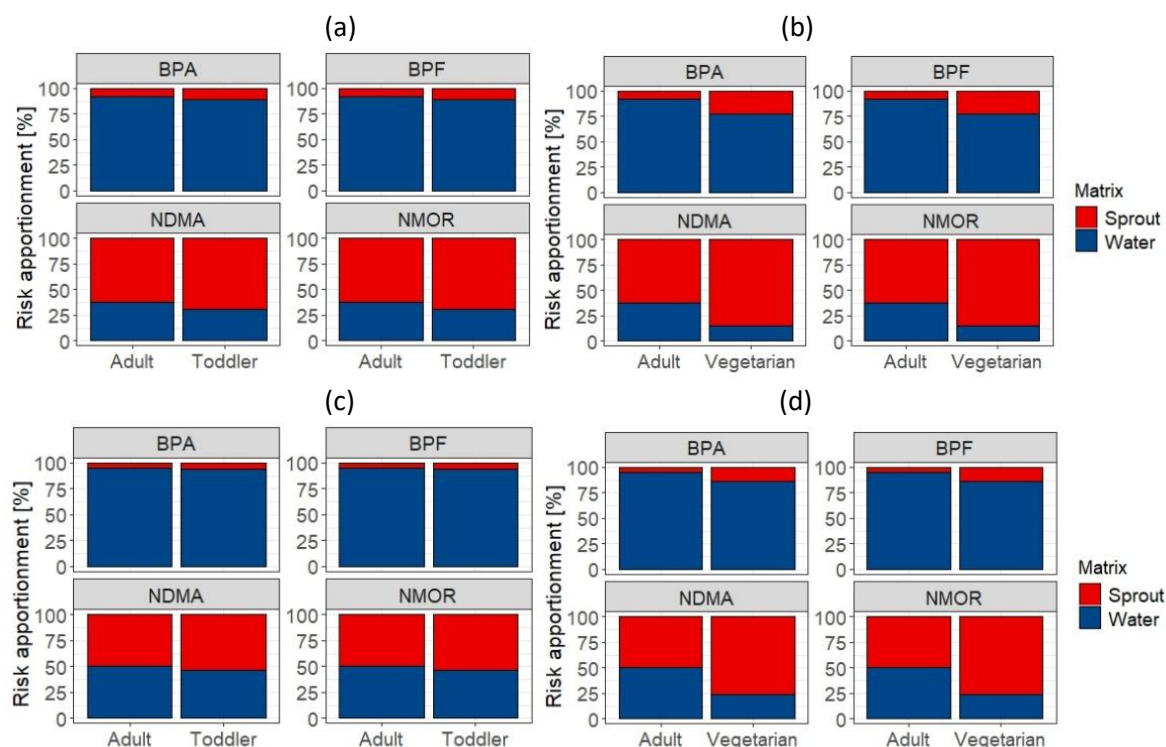


Figure 3-16: Risk apportionment when the contaminant concentration is set to their LOQ for (a, b) alfalfa and (c, d) radish sprouts, comparing omnivore adults and toddlers (a, c) and omnivore adults and vegetarian adults (b, d).

3.5. Recommendations for water quality monitoring in case of pipe relining

This work permitted the collection of useful data to support and guide future water quality monitoring campaigns in DWDNs.

Firstly, the literature review highlighted which are the substances that should be monitored. The list includes bisphenols (mainly BPA and BPF), aliphatic and aromatic amines, epichlorohydrin, BADGE, 2-EHGE, chlorophenols, chlorobisphenols and nitrosamines. Moreover, water macro-parameters, such as temperature, pH, hardness and alkalinity should be also monitored, since that can affect leaching. If applied, it is also fundamental to monitor the residual disinfectant, which play a relevant role in material deterioration and ageing, and in production of DBPs having leached compounds as precursors. Another useful set of parameters that should be monitored includes absorbance, fluorescence and toxicity, which could be useful to identify substances that cannot yet be specifically measured.

As done for the considered case-study, when a pipe is relined, before restarting operation, it should be washed multiple times until water complies with regulatory standards, especially in case disinfection is applied during the washing. Monitoring of targeted parameters during routine operation is also highly recommended, to promptly detect potential release due to aging or DBP formation. Based on the current experience, it is recommended to start the monitoring right after the start of operation, and to sample more frequently at the beginning of the campaign, at least once every two weeks, to check the actual effectiveness of the washing.

It is important to reduce the LOQ of the bisphenols and nitrosamines as much as possible, since these compounds can represent a risk for the consumers, directly for drinking water ingestion, and indirectly for home-grown vegetables irrigated with drinking water.



4. Water management tool for DBPs minimization in DWDNs

4.1. Water management tool description

4.1.1. General description

A water management tool was developed as a decision-support system to assist decision-making at both distribution network and treatment plant levels, with the aim of reducing potential health risks associated with drinking water consumption due to the occurrence of DBPs. It is specially developed for networks using sodium hypochlorite as disinfectant. The overall structure of the tool is illustrated in Figure 4-1.

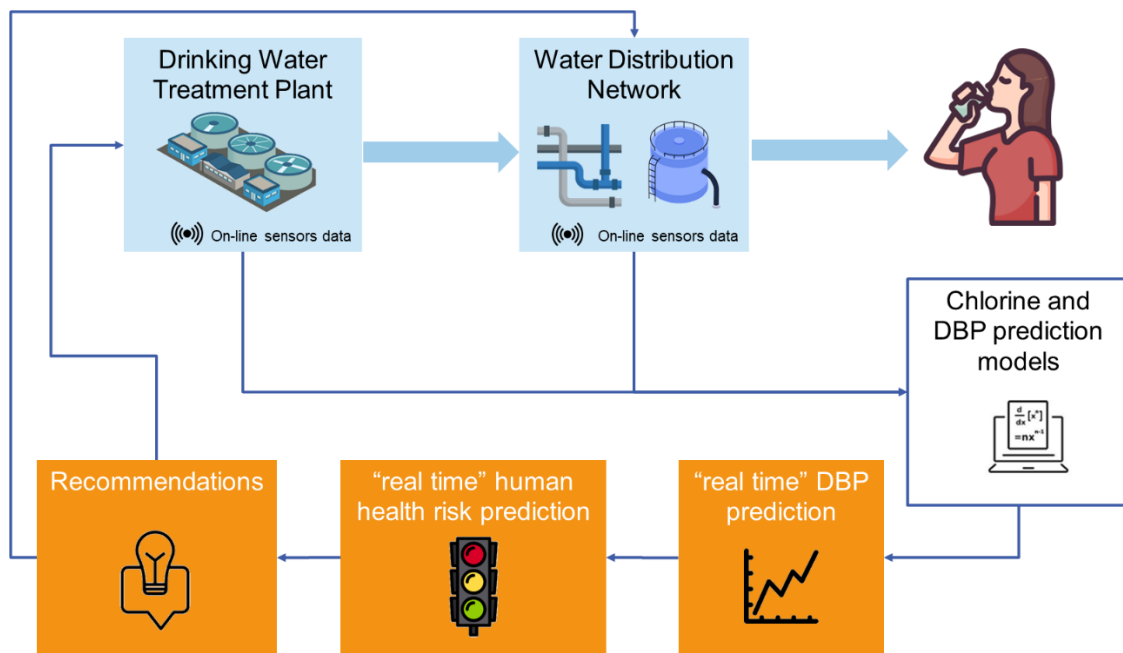


Figure 4-1: Water management tool scheme

The tool is fed with online data from sensors in the DWTP and the DWDN, including water temperature, chlorine doses applied during primary disinfection and at booster stations, free chlorine concentration, flow rates, tank volumes, valve status, and other water quality parameters. This data is used to estimate free chlorine and DBP concentrations at all points in the network using the mathematical models developed in Task 3.3 (as described in Deliverable 3.2). Based on these estimates, a risk assessment can be performed, and a risk index can be calculated for each point of the network. Finally, recommendations based on the predicted concentrations and associated risks can be generated to support decision-making at both plant and network levels, with the ultimate goal of complying with regulatory limits and reducing health risks associated with DBPs.

The following subsections describe the different components (modules) of this tool and the requirements that must be met by utilities wishing to implement it.



4.1.2. DBP prediction module

The modelling module of the tool operates based on the hydraulic model of the DWND. As input, it uses data from flow meters within the case study, water demand patterns, and the initial concentrations of the target compounds (e.g. at the outlet of the drinking water treatment plant), including free chlorine, trihalomethanes (THMs), haloacetic acids (HAAs), among others.

The modelling framework is implemented using EPANET, a widely used software tool for simulating the hydraulic and water quality behaviour of pressurised water distribution systems. This software enables the simulation of water residence times from the source to the point of interest, the decay of compounds such as free chlorine, and the formation of DBPs such as trihalomethanes.

Part of the CS#3 distribution network was hydraulically calibrated and validated in collaboration with CAT utility. Subsequently, data from sampling campaigns conducted by CAT in CS#3 were used to calibrate the DBP formation models within the study network. This process is described in further detail in Deliverable 3.2.

As outputs, this tool module provides estimations of individual THMs and HAAs at any of the hydraulically modelled points within the network.

It can be implemented for short-term estimations (e.g. daily or weekly) or for long-term predictions (months). For the latter, the integration of a demand forecasting model is required in order to identify consumption patterns within the network and anticipate future changes.

4.1.3. Human health risk assessment module

Risk module in the water management tool is based on the carcinogenic risk of THMs and HAAs which is the main long-term effect of DBPs.

Quantitative cancer risk assessment for chemical compounds is fundamentally based on integrating two core components: toxicity and exposure. Toxicity is characterized through dose–response relationships derived from epidemiological or animal studies, expressed as a cancer slope factor (SF) for oral and dermal exposure pathway and inhalation unit risk (IUR). SF and IUR represents the incremental increase in lifetime cancer risk per unit of chemical intake. On the other hand, exposure assessment estimates the magnitude, frequency, and duration of human contact with the contaminant. As explained in section 3.4.1, this involves calculating an ADD, taking into account compound concentration, rate of exposure to the compound (water consumption rates or inhalation rates), body weight, and exposure duration.

The quantitative cancer risk is then obtained by combining these two elements (equation 3.4). This yields an estimate of the probability of an individual developing cancer over a lifetime due to the specified exposure. In drinking water risk assessments, this framework allows regulators to establish guideline values or acceptable concentrations by back-calculating from target risk levels (e.g., 10^{-5} or 10^{-6}). The robustness of the assessment depends on the quality of both toxicity data and exposure assumptions, as well as the consideration of variability and uncertainty, which are often addressed through conservative assumptions or probabilistic methods.

In this work, exposure to DBPs was considered through two pathways: water ingestion and inhalation of vapours from water (shower scenario). Dermal contact was not considered, as it has been shown to be the pathway associated with the lowest risk compared to ingestion and inhalation (Ribera et al. 2014).



Since all countries that use water disinfection have already established legal limits for disinfection by-products (DBPs) based on risk assessment, complying with these limits generally ensures a safe level of exposure. However, because different compounds have different toxicity values, it is important to define water management strategies that not only meet regulatory limits but also minimize the overall chemical risk to the population.

For this reason, a new risk indicator was developed that is more intuitive than conventional cancer risk thresholds. This indicator ranges from 0 to 1 (representing no cancer risk and the maximum acceptable regulatory risk, respectively), making it easier to interpret and manage than values expressed in orders of magnitude. Equation 4.1 shows the concept for this normalized risk index (NRI). This index can be applied independently to each DBP family.

$$NRI = \frac{ILCR_{water}}{ILCR_{max}} \quad (4.1)$$

Where $ILCR_{water}$ is the increased life cancer risk of the water sample (at a specific point of the network and for a specific time) and the $ILCR_{max}$ is the increased life cancer risk of a water sample that contains the maximum allowed concentration of the most carcinogenic compound of the DBP family.

The decision of the most carcinogenic compound for each DBP family was made considering the combined risk of oral ingestion and inhalation of those compounds with defined SF and IUR. It was determined that BDCM and DBAA are the reference compounds for THMs and HAAs, respectively. Therefore, $ILCR_{max}$ was fixed at the cancer risk associated with a water composition that contained the maximum legally allowed concentration of BDCM or DBAA. In Spain, the legal limit for THMs is 100 µg/L and 60 µg/L for HAAs, then $ILCR_{max}$ would be the risk associated to 100 microg/L of BDCM or 60 microg/L of DBAA for the calculation of NRI_{THM} or NRI_{HAA} , respectively.

Table 4-1 shows the equations used for the calculation of ILCR for each exposure pathway and the total aggregated risk ($ILCR_{water}$). Table 4-2 presents the exposure parameters used in the equations. The inhalation pathway was defined as a showering scenario in which the volatilization factor from water to air for DBPs was obtained from Silva et al. (2013), who experimentally determined the volatilization ratios of THMs under controlled conditions (10-min shower, 40 °C water temperature, and a shower flow rate of 5.6-6-7 L/min). Table 4-3 summarizes the carcinogenic toxicity values used for each compound. It needs to be highlighted that not all compounds have available carcinogenic toxicity data for the exposure pathways considered.

Table 4-1: Equations used for human health risk assessment

Ingestion pathway	Inhalation pathway
For each DBP:	For each DBP:
$ADD = \frac{C_{water} \cdot IR \cdot EF \cdot ED}{BW \cdot AT \cdot 365} \quad (4.2)$	$C_{exp} = \frac{C_{water} \cdot VF \cdot ET \cdot EF \cdot ED}{AT \cdot 24 \cdot 365} \quad (4.3)$
For each DBP:	For each DBP:
$ILCR_{oral} = ADD \cdot SF \quad (4.4)$	$ILCR_{inhalation} = C_{exp} \cdot IUR \quad (4.5)$
Total risk considering all DBPs of the same family and all exposure pathways:	
$ILCR_{water} = \sum_{i=0}^{n_{DBP}} ILCR_{oral} + \sum_{i=0}^{n_{DBP}} ILCR_{inhalation} \quad (4.6)$	



Table 4-2: Exposure parameters used for human health risk assessment

Parameter	Value
IR – Water ingestion rate	2 L/day
EF – Exposure frequency	365 d/year
ED – Exposure duration	30 years
ET – Exposure time (shower)	10 min/day
BW – Body weight	70 kg
AT – Averaging time	83 years (lifetime expectancy in Spain)
VF – Volatilization factor from water in the shower (from Silva et al. 2013)	TCM: 6.29 ($\mu\text{g}/\text{m}^3$)/(mg/L) BDCM: 5.32 ($\mu\text{g}/\text{m}^3$)/(mg/L) TMB: 2.65 ($\mu\text{g}/\text{m}^3$)/(mg/L)

Table 4-3: Carcinogenic toxicity values used for human health risk assessment obtained from RAIS (<https://rais.ornl.gov/index.html>)

Compound	SF (mg/kg-day) ⁻¹	IUR ($\mu\text{g}/\text{m}^3$) ⁻¹
TCM	$3.1 \cdot 10^{-2}$	$2.3 \cdot 10^{-5}$
BDCM	$6.2 \cdot 10^{-2}$	$3.7 \cdot 10^{-5}$
DBCM	$8.4 \cdot 10^{-2}$	n.a.
TBM	$7.9 \cdot 10^{-3}$	$1.1 \cdot 10^{-6}$
MCAA	n.a.	n.a.
MBAA	n.a.	n.a.
TCAA	$7.0 \cdot 10^{-2}$	n.a.
DCAA	$5.0 \cdot 10^{-2}$	n.a.
DBAA	$2.5 \cdot 10^{-1}$	n.a.

n.a.: not available

Although this index provides an intuitive indication of the level of risk, it should be considered together with compliance with legal concentration limits. This is because not all regulated compounds exhibit carcinogenic toxicity via inhalation and ingestion, and it is possible for the NRI to be negligible while the total DBP concentration exceeds or equal the legal limit. For the illustration of different casuistic, two fictitious scenarios of water quality were calculated and represented in Figure 4-2. If scenario A is taken as reference (homogeneous concentration of the different compounds of the same family, and TTHMs and THAAs equal to the Spanish legal limits), the calculated NRI can be very different if the DBPs distribution is different. In scenario B (same TTHMs and THAAs than scenario A but different distribution), NRI_{TTHM} is higher and NRI_{HHA} is lower than in scenario A.

Therefore, the water management tool includes both the evaluation of the DBP concentrations and the two NRI.



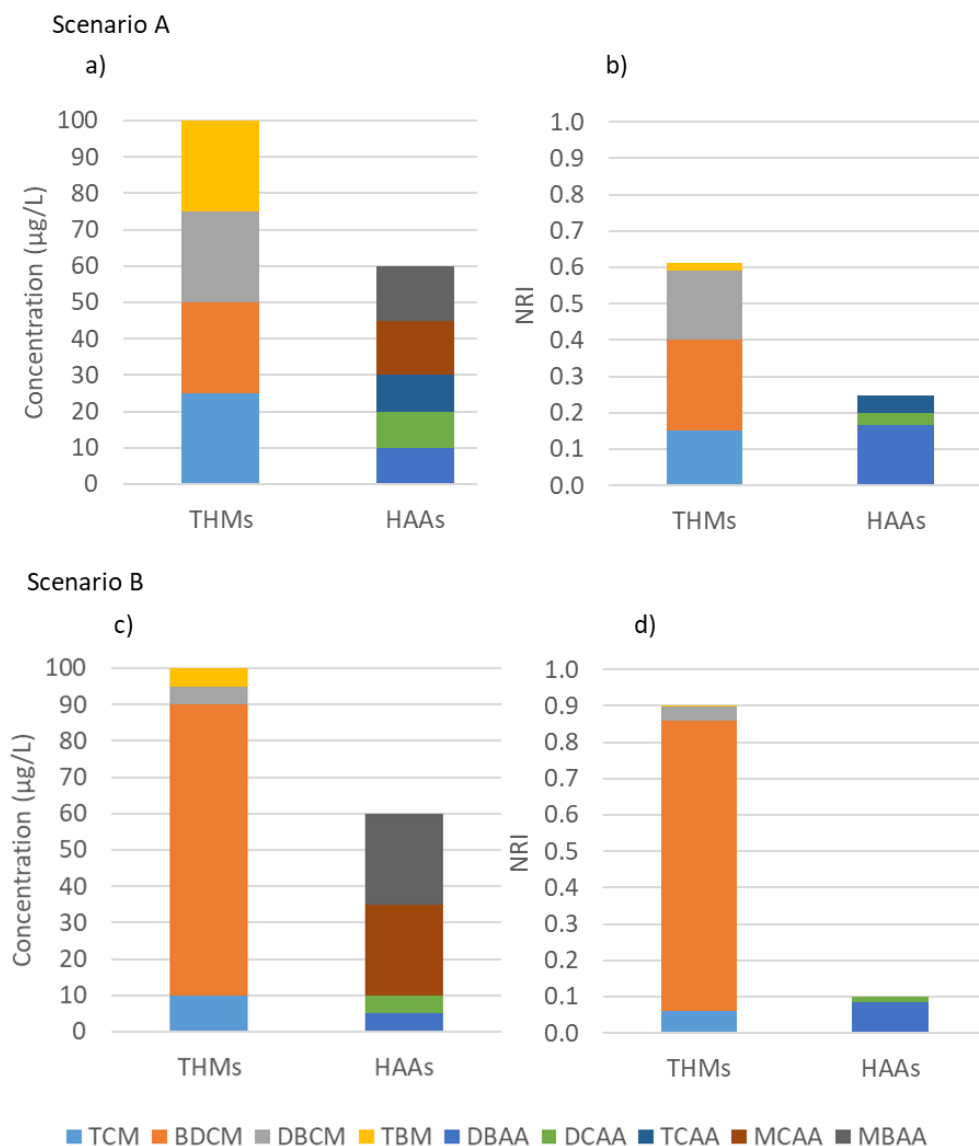


Figure 4-2: DBPs concentrations (a, c) and corresponding NRI (b, d) for two fictitious scenarios. Scenario A (a, b) and scenario B (c, d).

4.1.4. Recommendations module

Within the water management tool, the decision-support module must be tailored to each case study, as final decisions need to account for existing processes in the DWTP and the available control elements in the DWDN.

This section outlines a range of potential actions that can be implemented at both the DWDN and DWTP levels. For each case study, however, the feasibility and effectiveness of these actions should be carefully assessed to identify the most appropriate strategy. Some of the recommendations are easily implemented (e.g. reducing tank residence time) but others might require some time for planning (e.g. flushing of pipes) or investments (e.g. addition of a NOM removal process in the DWTP).

In addition, the analysis of historical data can support the identification of periods with higher DBP formation potential, enabling a more targeted and proactive implementation of mitigation measures.



For example, periods with elevated NOM concentrations in source water (e.g. during low river flow conditions in surface water systems) may require the application of specific control strategies. Recommendations are detailed in Table 4-4.

Table 4-4: Recommended actions for high DBP concentration or high-risk cases

Goal	Recommendations
Reduce water age	• Optimize valve operations. • Eliminate dead-ends or low-flow areas. • Reconfigure sectors to increase circulation. • Review network extremities and low-demand zones.
Optimize storage tank operation	• Reduce unnecessary storage volumes. • Improve internal mixing. • Avoid thermal stratification. • Adjust minimum and maximum levels to increase turnover
Implement target flushing	• Carry out scheduled flushing in areas with high water age or elevated DBPs. • Prioritize dead-ends, low-demand zones, and oversized pipes.
Control disinfectant residual	• Avoid overdosing at chlorination boosting stations. • Adjust setpoints based on demand, temperature, and residence time. • Maintain sufficient but not excessive residual levels. • Redefine location of chlorination boosting stations • Redefine disinfection process in some chlorination boosting stations
Improve network cleaning and maintenance	• Remove accumulated sediments. • Control biofilm and scaling. • Prioritize older pipes or those with low flow velocities.
Manage seasonal variations	• Apply specific seasonal strategies to prevent increase of DBPs in most problematic seasons. • Activate extra treatment processes or increase efficiency of existing ones in the DWTP.
Improve DWTP efficiency in NOM removal	• Increase chemical usage in some processes (e.g. optimisation of coagulant and/or oxidant dosing). • Activate or implement extra treatment processes or duplicated lines. • Modify water sources (in case different water sources are available).

4.1.5. Requirements for water tool implementation

To enable the implementation of the water management tool developed and shown here, these are the requirements that the system needs to fulfil:

- Availability of online monitoring systems, including flow meters, tank level sensors, free chlorine concentration, and, optionally, DBPs sensors (inline THMs).
- A calibrated hydraulic model of the distribution network, suitable for performing simulations using hydraulic solvers such as EPANET. If this is not fulfilled, the hydraulic model will be developed previously to the tool implementation.
- Sampling campaigns targeting the DBPs to be estimated, conducted at different locations within the network, including the determination of initial concentrations. This is required to calibrate some of the water quality model parameters.

4.2. Water management tool implementation in CS#3

This tool was developed specifically for CS#3 (Tarragona, Spain). Although it could not be fully implemented within the SafeCREW timeframe due to the incomplete availability of the hydraulic model, its deployment is planned in the coming months once the utility (CAT) finalizes the integration of the hydraulic digital twin into its control system. Nevertheless, an offline application was carried out



and is presented in this section, especially the results for the risk assessment module, since results of the prediction module are already shown in Deliverable D3.2.

The calculation of the normalized risk associated with THMs and HAAs provides an overall assessment of the DWDN status. One possible visualization is the mapping of the normalized risk index (NRI) at different locations within the network, to identify critical areas and implement mitigation measures if necessary.

Figure 4-3 shows an example of the visualization maps for human health risk using the defined NRI applied to CS#3. These maps were developed with data from 2025 (January for winter, May for spring, August for summer and October for autumn). Data used for the creation of these maps are available in Zenodo (10.5281/zenodo.19890063).

The lowest risk levels are observed in spring, followed by winter, summer, and finally autumn. Spring presents the most favourable conditions due to lower temperatures and improved source water quality associated with snowmelt. In contrast, autumn exhibits the least favourable conditions in terms of DBP formation, mainly due to higher temperatures and reduced river flow, which leads to increased concentrations of organic and inorganic matter, acting as precursors for DBPs. In addition, higher temperatures require higher disinfectant doses to maintain the residual chlorine necessary to ensure microbiological safety.

Within the same network, points located farther from the DWTP tend to have higher NRI. In particular, *Sant Jaume dels Domenys* shows the highest DBPs levels, likely due to the combination of longer residence times and its location within the network, where multiple chlorine booster stations points contribute to increased disinfectant dosing.

This information, together with the concentration evolution of each DBP in the network supplied by the same water management tool will provide the operators with the capacity to take decision on the network management with the aim to minimize risk and optimize energy and chemicals consumption.

4.1. Online web tool: DBP Risk Explorer

Building on the developments carried out for the creation of the water management tool, an online web-based application (named *DBP Risk Explorer*) was developed to enable utilities to generate preliminary estimations of DBP concentrations and the associated risk levels throughout the distribution network. This tool is designed as an initial decision-support resource, allowing users to visualize and assess potential water quality issues in a simplified and accessible environment.

The main objective is to provide utilities with a practical demonstration of the added value of integrating an online water management tool into their operational systems. By interacting with the platform, users can explore different scenarios and better understand how such tools can support proactive management strategies, enhance risk assessment capabilities, and ultimately contribute to more informed and timely decision-making processes.

The tool is a web-based application that enables the simulation of free chlorine and selected DBPs, including THMs, HAAs, haloacetonitriles (HANs), and chlorate. The results are based on simulated scenarios and provide an indicative assessment of the expected behaviour under specific conditions, such as water source characteristics and the type of disinfectant applied. The website is open and available on [DBP Risk Explorer](#).



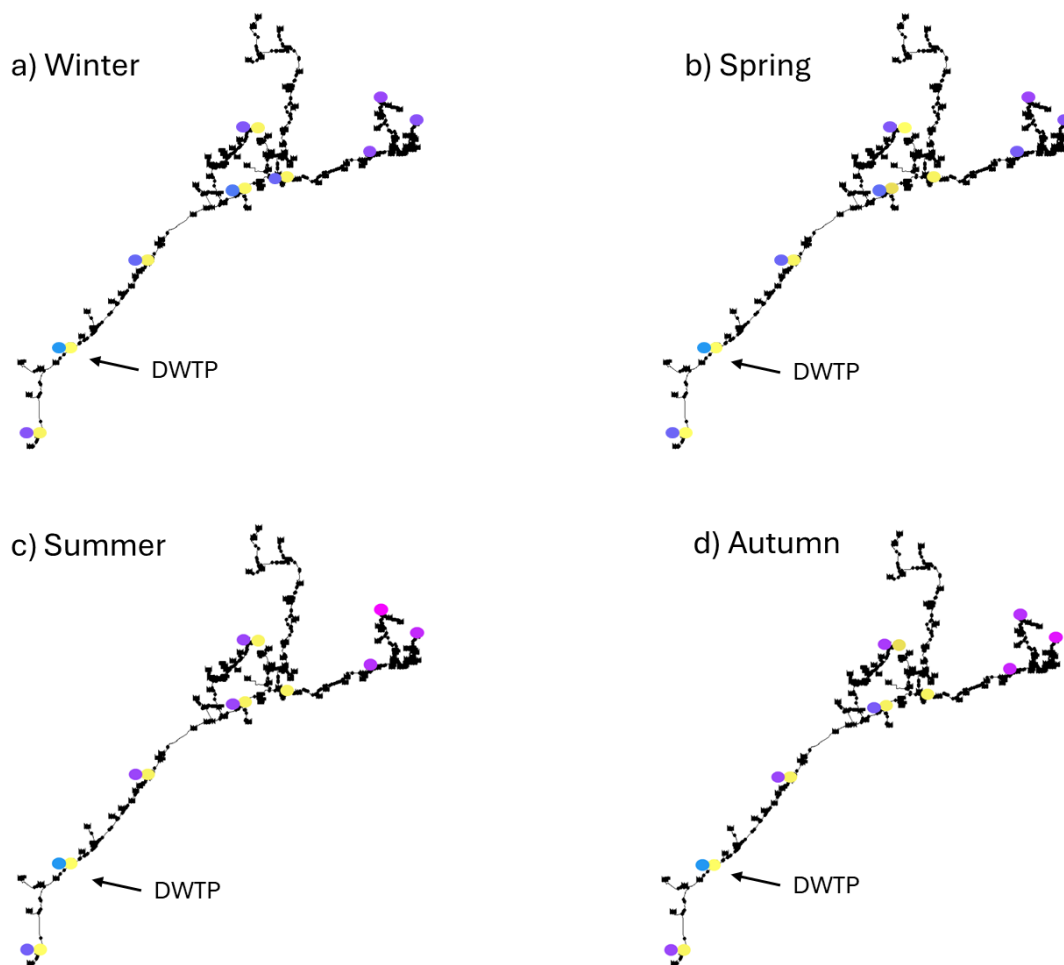


Figure 4-3: THMs normalized risk index in the CS#3 distribution network at different seasons: (a) winter, (b) spring, (c) summer, (d) autumn

Figure 4-4 presents the initial screens of the web application. The first screen corresponds to the landing page. The second screen prompts the user to specify the country and the type of entity (for statistical purposes only). The third screen allows the user to select the family of DBPs to be simulated.

When THMs, HHAs or HANs are selected, the user needs to provide information about the chlorine decay in the network or use default data (derived from CS#3) (see Figure 4-5) and then provide information about the DBP family that needs to be simulated: initial concentration and formation potential (except for HANs). This can be seen in Figure 4-6 for THMs, Figure 4-7 for HHAs and Figure 4-8 for HANs.

Then, the web application returns graphical representation of chlorine decay through the network and individual DBP evolution. It also provides the evolution of the NRI for THMs and HHAs.

The case of chlorate differs from other DBPs, as its concentration does not primarily evolve within the distribution network but rather in the storage tanks containing concentrated hypochlorite (used for primary or secondary chlorination). In this context, the web application estimates the temporal evolution of chlorate concentration within the hypochlorite storage tank (see Deliverable 3.2 for further details).



This functionality is particularly relevant for assessing the contribution of chlorate to the network as a result of hypochlorite degradation during storage, as well as for identifying and implementing strategies to minimize disinfectant decay.

For this estimation, the tool requires the following input parameters: initial hypochlorite concentration, storage tank volume, and the chlorine dose applied to the water (i.e., at the outlet of the hypochlorite storage tank) (see Figure 4-9). It should be noted that the simulation assumes a closed system and does not account for tank refilling with fresh disinfectant; instead, it only considers the storage and dosing processes over time.

DBP Risk Explorer

On-line simulator to predict DBPs formation and associated risk in drinking water distribution networks based on simple models and minimum number of input parameters

While the tool does not aim to accurately predict all DBPs at all locations, it offers a useful indication of potential risks that warrant further analysis. It also facilitates understanding how factors such as temperature and water residence time affect DBP formation.

Start

safe CREW **eurecat**

Country

Spain

Authority / regulatory body
Type of entity

University or research institute

Information requested for statistical purposes only

Continue

Which DBP do you want to evaluate?

☐ THMs

☐ HAAs

☐ HANs

☐ Chlorate

Continue

Figure 4-4: Initial screens of the “DBP Risk Explorer” web tool



Free Chlorine Decay Simulation

Fill in according to the information you have from your network:

☐ Free chlorine decay constant is equal to: 1/h

☐ After h (RT2) free chlorine decays mg/L

☐ I don't have any information. I want to estimate free chlorine decay at °C

Minimum legal = Maximum legal = mg/L (Spain: 0.2 - 1 mg/L)

Initial free chlorine * mg/L

Simulation of residence time * h This is the time between two points in the network (water path)

Continue

Figure 4-5: Free chlorine input data screen of the “DBP Risk Explorer” web tool

THMs

Initial TCMs:	TCMFP:
Initial BDCMs:	BDCMFP:
Initial DBCMs:	DBCMFP:
Initial TBMs:	TBMFP:

Legal limit TTHMs: µg/L

Continue

Figure 4-6: THMs input data screen of the “DBP Risk Explorer” web tool



The screenshot shows a web form titled "HAAs" for inputting data. It contains two columns of input fields. The left column has five fields labeled "Initial THAAo:", "Initial BCAAo:", "Initial DBAAo:", "Initial DCAAo:", and "Initial TCAAo:", each followed by a unit of $\mu\text{g/L}$. The right column has five corresponding fields labeled "THAAFP:", "BCAAFP:", "DBAAFP:", "DCAAFP:", and "TCAAFP:", each followed by a unit of $\mu\text{g/L}$. Below these columns is a single field labeled "Legal limit HAAs:" followed by a unit of $\mu\text{g/L}$. At the bottom center is a blue button labeled "Continue".

Figure 4-7: HAAs input data screen of the “DBP Risk Explorer” web tool

The screenshot shows a web form titled "HANs" for inputting data. It features a section labeled "Input data:" with a single input field labeled "Initial HAN concentration" containing the value "0", followed by a unit of $\mu\text{g/L}$. At the bottom are two buttons: a grey "Back" button and a blue "Continue" button.

Figure 4-8: HANs input data screen of the “DBP Risk Explorer” web tool



Figure 4-9: Chlorate input data screen of the “DBP Risk Explorer” web tool

To illustrate the outputs provided by the DBP Risk Explorer web application, a series of simulations were performed based on the data presented in Table 4-5. Output screens are shown in Figure 4-10 for free chlorine, Figure 4-11 for THMs, Figure 4-12 for HAAs, and Figure 4-13 for chlorate. Furthermore, the web application allows the user to download the simulation results in pdf format.

Table 4-5: Input data used to create the example simulations of the “DBP Risk Explorer” web tool.

Parameter	Value
Parameters for chlorine simulation	Initial free chlorine = 1,5 mg/L Chlorine decay constant = 0,014 1/h
Residence time	24 h
Legal limit	THMs: 100 µg/L HAAs: 60 µg/L
Initial concentration	THMs: 0 µg/L for TCM, 5 µg/L for BDCM, 5 µg/L for DBCM and 0 µg/L for TBM HAAs: 0 µg/L for all HANS: 0 µg/L for all
Formation potential	THMs: 30 µg/L for TCM, 20 µg/L for BDCM, 40 µg/L for DBCM and 15 µg/L for TBM HAAs: 10 µg/L for BCAA, 6 µg/L for DBAA, 15 µg/L for DCAA and 10 µg/L for TCAA
Hypochlorite storage tank information	Initial sodium hypochlorite concentration: 180 g/L Volume: 50 L Outlet flowrate: 1 L/h



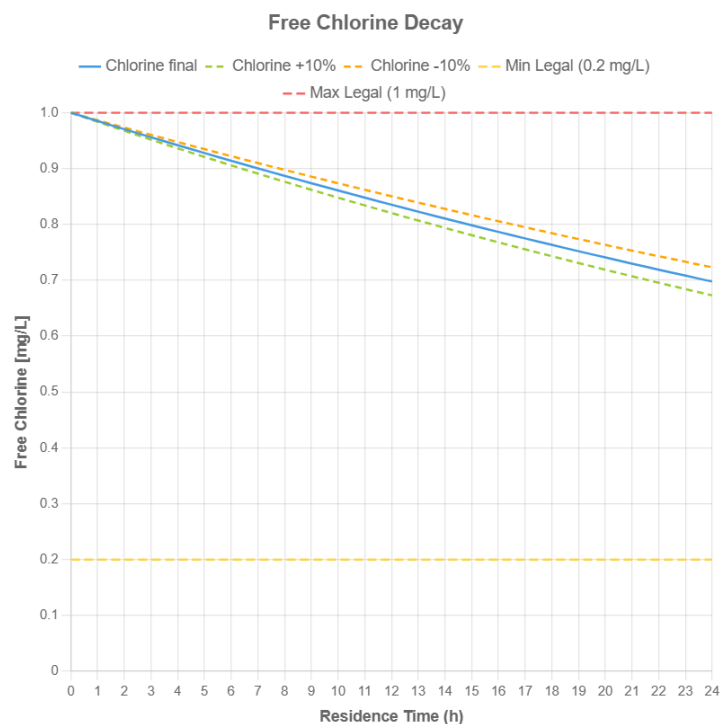


Figure 4-10: Free chlorine decay over time calculated by the “DBP Risk Explorer”.

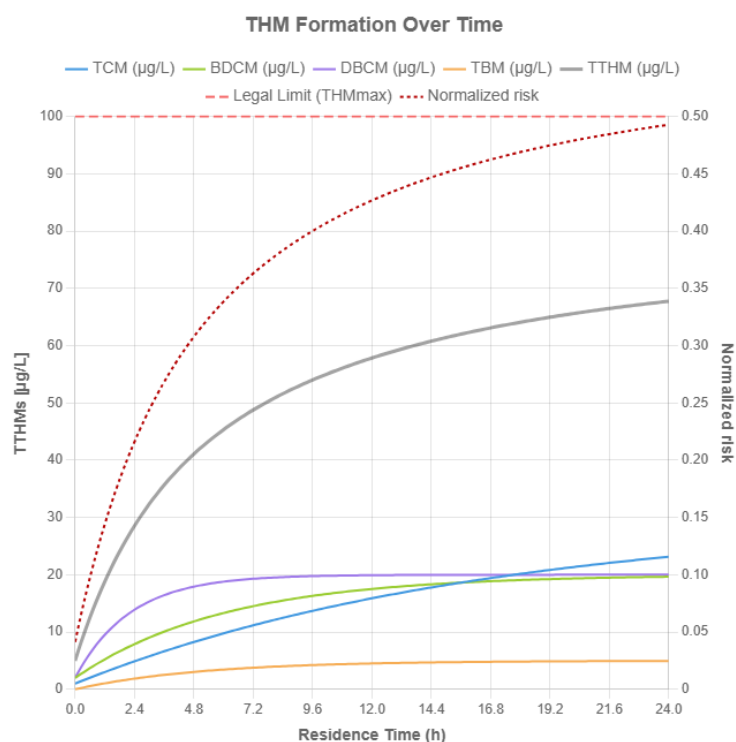


Figure 4-11: THMs concentration and associated risk over time calculated by the “DBP Risk Explorer”.



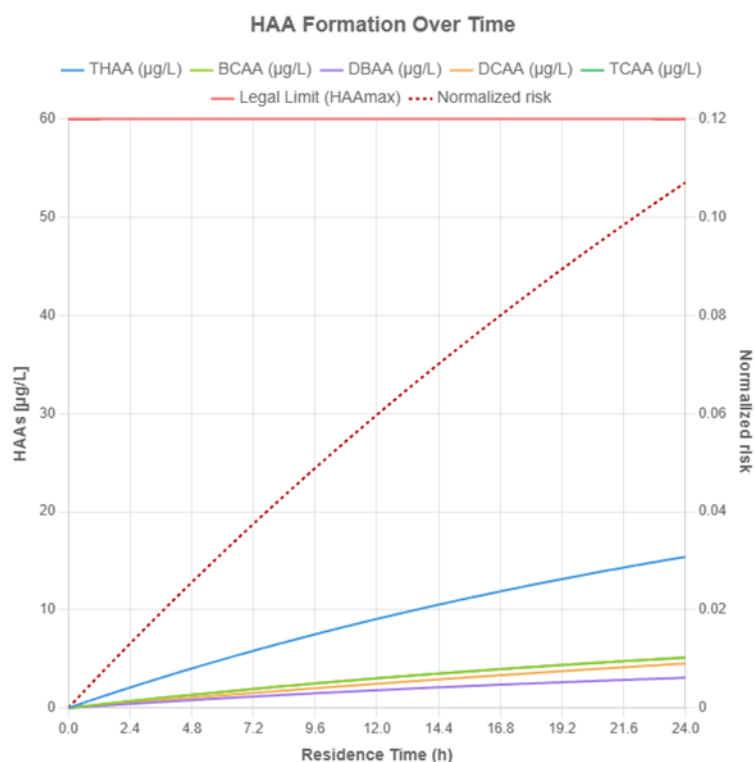


Figure 4-12: HAAs concentration and associated risk over time calculated by the “DBP Risk Explorer”.

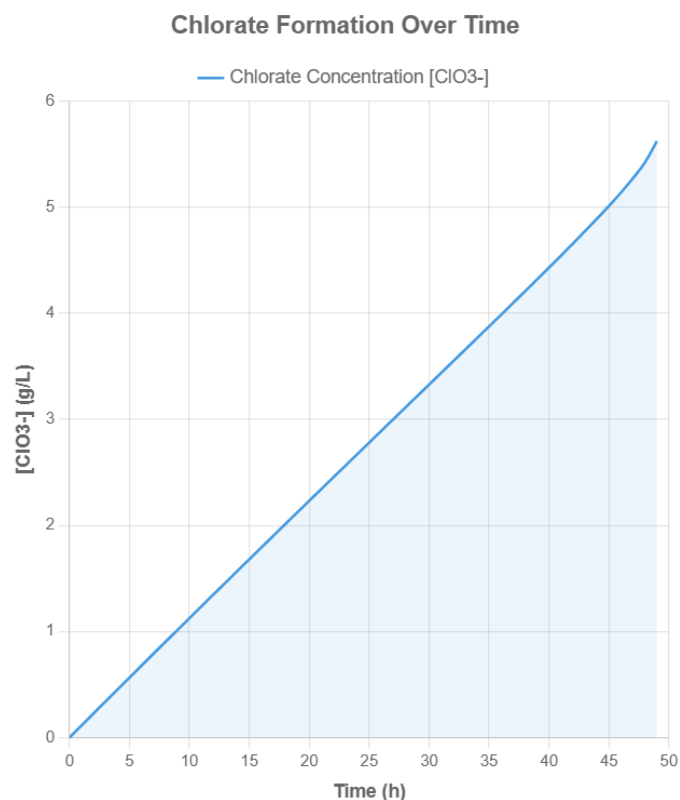


Figure 4-13: Chlorate concentration evolution over time in the hypochlorite storage tank calculated by the “DBP Risk Explorer”.



5. Conclusions

This deliverable provides an integrated assessment of water quality monitoring and DBP management in drinking water distribution networks (DWDNs), focusing on pipe repair impacts and operational decision-support. The main conclusions are:

- Materials and relining processes are relevant sources of contaminants and DBP precursors. Substances released from pipes, particularly from polymers and epoxy resins, can contribute to DBP formation.
- Pipe relining can temporarily deteriorate water quality. The CS#2 case study showed increases in organic matter and DBPs after relining, especially in early operation, while flushing was effective but not sufficient for all compounds.
- Nitrosamines are key compounds of concern. They were the most consistently detected and require targeted monitoring due to their persistence and toxicity.
- Monitoring should combine targeted and non-targeted indicators. Parameters such as TOC, fluorescence, and toxicity complement chemical analyses and improve risk detection.
- Risk assessment should include indirect exposure pathways. While drinking water is the main route, plant uptake can contribute to exposure for specific contaminants.
- Current analytical limits may underestimate risk. Exceedances at LOQ levels highlight the need for more sensitive analytical methods.
- The developed water management tool supports proactive management. By integrating modelling and risk assessment, it enables estimation of DBPs and associated risks across the network using an intuitive normalized risk index.
- DBP risks vary across space and time. Higher risks are linked to longer residence times, higher temperatures, and network extremities, as shown in CS#3.
- Operational measures can reduce DBPs effectively. Strategies such as reducing water age and optimizing disinfection are essential.
- The proposed approach enables a shift to risk management. It supports utilities in moving beyond compliance towards proactive control aligned with EU objectives.

This work contributes to climate-resilient and risk-based management of drinking water systems by:

- Advancing understanding of combined effects of infrastructure materials and disinfection processes.
- Providing validated methodologies and tools for monitoring and risk assessment.
- Supporting utilities in moving from compliance-based to proactive, risk-informed management.
- Addressing emerging concerns related to low-level contaminants and indirect exposure pathways.

The developed framework and tools are transferable across European DWDNs, offering practical support for utilities facing increasing regulatory and environmental pressures.



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