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Review of modelling solutions for intoDBP

Deliverable 3.1

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Author: Pavlos Pavlou

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ABSTRACT	This deliverable will summarize the findings from reviewing existing modelling tools, software, and procedures to model the formation of DBPs in water distribution networks. The analysis will focus on open-source software and published results and identify their key features and licensing status. Selected state-of-the-art methodologies, most relevant for optimal control and minimization of DBP-related risks, will be studied. These methodologies include state estimation, optimal sensor placement, DBP formation prediction through UV-VIS and fluorescence signal analysis measuring the reduction of DOM (DBP precursors), early warning detection and decision-making tools.		

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EXECUTIVE SUMMARY

Monitoring disinfection by-products (DBPs) in drinking water is challenging due to the need for regular sampling and advanced equipment. Further, modelling DBPs in water networks is complex. For Digital Twins to be of assistance, calibrated DBP models and real-time data integration are required. Challenges include acquiring accurate data, dealing with chemical dynamics, and model validation. This overview provides the latest insights into DBP modelling, emphasizing methodologies for prediction, control, and risk reduction, including sensor placement and early detection.

DBP formation is affected by factors such as the type of disinfectant, pH levels, temperature, and the presence of organic or inorganic components. Water network properties like velocity, retention time, water age, and pipe material also impact DBP formation. Water stagnation can increase DBP levels while biofilms affect chlorine levels and DBP formation. Further research is needed to understand flow-dependent DBP kinetics and material effects on different DBP families.

Three spectroscopy methods are suggested for monitoring DBPs. UV-Vis spectroscopy measures organic matter absorption of UV and visible light but its reliability can be affected by factors such as pH, and iron Fluorescence spectroscopy analyzes dissolved organic matter through fluorescence properties. This is rapid, sensitive, and suitable for real-time DBP monitoring, though diverse DOM compositions pose challenges. Biosensors, including electrochemical sensors utilize biological recognition elements for detection and they are promising for DBP monitoring due to speed and affordability.

Models for studying DBPs can be classified as Static Variable (SV) models, using fixed inputs except for time, or Dynamic Variable (DV) models, which rely on changing variables due to disinfection. SV models utilize regression methods, mechanistic approaches and artificial intelligence (AI). These models are mainly applied to THMs and HAAs and are based on laboratory or full-scale data, often focusing on raw water. DV models relate DBPs to changes in water properties during disinfection. They often express these changes differentially, presenting variance between initial and subsequent values.

Sensor placement strategies have mainly focused on finding the best locations to monitor contamination events and common water quality factors. However, there's a lack of research on sensor placement for DBPs, especially when using alternative disinfectants like chlorine dioxide and chloramine and utilizing modern sensor data like UV and DOM measurements.

This review highlights the need for more research focusing on DBP formation within WDN, improved replication of organic matter, a balanced focus on different DBP classes, and a shift toward mechanistic models. Further, it's important to keep dynamic models simple when simulating DBP formation because considering all dynamic variables is impractical. Despite efforts to improve accuracy, ongoing research is necessary to make these models work in different situations and water systems.

1.0 INTRODUCTION

1.1 Disinfection and disinfection by-products

Producing safe and potable tap water is a crucial public health service provided by drinking water authorities and utilities. The disinfection of drinking water to reduce waterborne diseases is widely recognized as the most significant public health accomplishment of the 20th century (Sedlak & von Gunten, 2011). Several chemical disinfectants are utilized for water disinfection including chlorine (e.g., in the form of hypochlorous acid, HClO), chlorine dioxide (ClO_2), chloramine (NH_2Cl), ozone and UV radiation (WHO, 2017a). These compounds can effectively eliminate various pathogenic bacteria and conditional pathogens. However, they can react with both organic (natural and anthropogenic) and inorganic compounds (bromide, Br-, or iodide, I-) in the water, producing Carbonaceous and Nitrogenous Disinfection By-Products (C-DBP and N-DBPs) that are considered undesirable, as many of these DBPs can be harmful to human health, with teratogenic, carcinogenic, and mutagenic effects (Maeng et al., 2019). Regarding chlorine dioxide, the existence of both organic and inorganic components can lead to the creation of inorganic chlorite which can then transformed into chlorate ions (Kurajica et al., 2020; Sathasivan et al., 2020).

As a result, global drinking water standards have imposed strict regulations on the presence of DBPs in drinking water. Currently, over 700 types of DBPs have been detected in drinking water, but only a handful are subject to regulations (Dong et al., 2023; Fang et al., 2022; Kali et al., 2021). The EU's Drinking Water Directive (DWD) sets the maximum allowable level for THMs and HAAs at 100 µg/L and 60 µg/L, respectively (The European Parliament and the Council of the European Union, 2020). Canada has set the maximum permissible limit for HAAs at 80 µg/L while Nigeria has established a maximum allowable limit of 1 µg/L for THMs. Other countries have regulated DBPs including USA (US EPA), South Africa ("South African Bureau of Standards," 2015), Australia (National Health and Medical Research Council, 2011) and Singapore (Board, 2022). **Table 1 lists the three most used disinfectants and their potential DBPs in water distributions networks (WDN), namely, chlorine, chloramine and chlorine dioxide.** It is important to note that the maximum allowable level of DBPs can vary depending on the type of standard used. In the present report, we consider two sources in this field, namely the World Health Organization (WHO) (WHO, 2017b) and the European Union (The European Parliament and the Council of the European Union, 2020). Regarding DBP-related diseases, it should be emphasized that human studies have not been conducted on many of the DBPs compounds. Consequently, this report relied on papers that reported results on health whether they were conducted in vivo or in vitro.

Table 1: Comparison of disinfection by-products formed by different disinfectants including regulatory status, guidelines and related diseases.

Disinfectant	DBP	Group Name	Regulatory Status	Standard Value(µg/l)		Cancer Group (IARC)	Related Diseases	References
				EU	WHO (Guideline)			
Chlorine (Hypochlorous Acid)	THMs	Chloroform	Regulated	100 for total THMs	300	2Bb	Bladder cancer, colorectal cancer, adverse birth outcomes	(Kali et al., 2021; H. Zhang et al., 2018)
		Bromodichloromethane			60	2B		
		Dibromochloromethane			100	Not classified		
		Bromoform			100	3c		
	HAAs	Bromoacetic acid	Regulated	60 for total HAAs	-	2B	Bladder cancer, liver cancer	(EPA, 1998; H. Zhang et al., 2018)
		Chloroacetic acid			-			
		Dibromoacetic acid			-			
		Dichloroacetic acid			-			
		Trichloroacetic acid			50			
		Dibromochloroacetic acid	Unregulated		200			
		Bromochloroacetic acid			-	Not classified		
		Bromodichloroacetic acid			-	2B		
		Tribromoacetic acid			-	Not classified		
					-	Not classified		

Disinfectant	DBP	Group Name	Regulatory Status	Standard Value(μg/l)		Cancer Group (IARC)	Related Diseases	References
				EU	WHO (Guideline)			
Chlorine Dioxide	Inorganic DBPs	Chlorite	Regulated	250	700	3	Anemia, the nervous system effects	(Bull et al., 2009; Kurajica et al., 2020)
		Chlorate	Regulated	250	700	Not classified	Thyroid disruption	(Bull et al., 2009)
Chloramine	Haloacetaldehydes	Chloral hydrate	Unregulated	-	-	2Ad	Liver cancer	(Postigo et al., 2017)
	Nitrosamines	Nitrosodimethylamine	Unregulated	-	0.1	2A	Bladder cancer, pancreatic cancer	(Gan et al., 2013; Hrudey et al., 2015; H. Zhang et al., 2018)
		Nitrosodibutylamine		-	-	NONE		
		Nitrosodi-n-propylamine		-	-	2B		
		Nitrosomethylethylamine		-	-	2B		
		Nitrosodiethylamine		-	-	2A		
		Nitrosopyrrolidine		-	-	2B		
		Nitrosodiphenylamine		-	-	2B		
		Nitrosodiphenylamine		-	-	3		
		Nitrosomorpholine		-	-	2B		
	HANs	Dichloroacetonitrile	Unregulated	-	20	3		

Disinfectant	DBP	Group Name	Regulatory Status	Standard Value(µg/l)		Cancer Group (IARC)	Related Diseases	References
				EU	WHO (Guideline)			
		Trichloroacetonitrile		-	-	3	Reproductive and developmental effects, liver and kidney effects	(Richardson et al., 2007)
		Bromochloroacetonitrile		-	-	3		
		Dibromoacetonitrile		-	70	2B		

[a] International Agency for Research on Cancer, (1972-present)

[b] Possibly carcinogenic to humans

[c] Not classifiable as to its carcinogenicity to humans

[d] Probably carcinogenic to humans

1.2 Challenges

There is a constant fluctuation in the types and concentrations of DBPs within WDNs, with the regulated DBPs typically present at higher levels than those found in WTP effluent water (Dong et al., 2022). Further, the formation of DBPs is influenced by various factors, including the characteristics of the source water such as the concentration and type of organic matter, pH, temperature, type and concentration of disinfectants, contact time, point of addition, etc.(Chhipi-Shrestha et al., 2018; Plewa et al., 2017). Thus, due to the complex interplay between the probability of different DBP formation pathways during disinfection and their subsequent transformation within the distribution network, their study and monitoring are challenging. Although there is partial insight into the toxicity of individual DBPs, only a few data are available regarding the toxicity of DBP mixtures and the prolonged consequences of exposure to low DBP levels. This deficiency in information can complicate the precise evaluation of health hazards linked to DBP exposure and pose hurdles in establishing regulatory thresholds (Qadafi et al., 2023)

1.2.1 Monitoring DBPs through sampling and online field sensors

The process of monitoring DBPs in drinking water involves regular sampling and analysis of collected samples. Water sampling data is considered the most reliable information for evaluating water quality, however, for many water operators, frequent water sampling and analysis of various water quality parameters can pose a challenge due to technical, financial, and infrastructural limitations. Moreover, most emerging DBPs are present in drinking water at very low concentrations (e.g., <5 µg/L), which requires advanced analytical instruments and experienced technicians for accurate quantification. The analysis of emerging DBPs can also be costly, making it an unviable regular practice for many water utilities (G. Hu et al., 2023; Z. Xu et al., 2022).

Effective control of DBPs in WDNs requires real-time adjustments to the primary and secondary disinfection operations (e.g., disinfectant dosages). This cannot be achieved without a sensor-based monitoring system that provides real-time water quality data. Although various sensors have been developed for real-time monitoring of water quality parameters that could represent or be surrogated for conventional DBPs there is a significant lack of sensors specifically designed for monitoring emerging DBPs (Sadiq & Rodriguez, 2004; Wu et al., 2019; Zeng et al., 2019; C. Zhang & Lu, 2021).

1.2.2 Modelling DBPs in water distribution networks

Given the complexity of DBP formation, a multi-faceted approach is required to effectively monitor and control their levels. Digital Twins provide a virtual replica of the WDN and can be a valuable tool for analyzing DBPs. However, the incorporation of DBP models along with the integration of real-time data from field sensors are essential for a digital twin to accurately simulate the formation and fate of DBPs with a WDN. If achieved, this technology enables water utility managers to gain a deeper understanding of DBP dynamics, assess the effectiveness of treatment strategies, and

respond proactively to fluctuations in water quality, such as those caused by climate change. Climate change can exacerbate the formation of DBPs due to changing water source quality and temperature, among other factors. Ultimately, effective management of DBPs requires a comprehensive understanding of the complex interactions that lead to their formation and the use of advanced modelling and simulation tools. The development of accurate and reliable models for DBP formation and control can contribute to the development of more effective strategies for managing DBPs and ensuring the safety of drinking water.

Some of the main challenges affecting the accuracy of the modelling procedure are listed below:

- **Availability of accurate and comprehensive model input data:** The availability of data on water hydraulic and quality parameters and disinfection conditions significantly influences the accuracy of DBP models. To create precise models, it is crucial to gather representative data from different sources. While certain researchers have made efforts to investigate these factors (Bagheban et al., 2019), it's worth noting that certain crucial parameters such as precursor concentrations and disinfection kinetics may pose challenges in terms of accessibility (Z. Xu et al., 2022).

- **Complexity and uncertainty of chemical dynamics:** The modelling process requires an accurate representation of the relevant chemical reactions and physical processes. Additionally, uncertainty in model parameters can affect the accuracy of risk assessments and lead to uncertainty in model predictions. Parameters such as reaction rate constants can be difficult to accurately measure and vary depending on the water source and treatment processes (G. R. Abhijith & Ostfeld, 2022a; Kulkarni & Chellam, 2010).

- **Model validation:** It can be challenging to validate DBP models due to the lack of real field data on DBP formation under different conditions. In addition, there are often discrepancies between laboratory-scale experiments and full-scale systems, which can make it difficult to extrapolate model predictions to real-world scenarios (Chowdhury et al., 2009).

1.3 Scope

This deliverable aims to provide a comprehensive and up-to-date overview of the current state of knowledge on **DBP formation modelling in WDN**, with a focus on recent advancements in the field. It will also summarize the findings from reviewing existing modelling tools, software, and employed procedures. The analysis will emphasize state-of-the-art methodologies crucial for predicting, controlling, and minimizing DBP-related risks, including state estimation, optimal sensor placement, DBPs formation prediction, early warning detection systems, and decision-making tools.

This deliverable is organized as follows. In Section 2, the factors affecting DBP formation are described. Information on existing sensing technologies is provided in Section 3. We summarize the DBP modelling approaches in Section 4 while in Section 5 we provide an overview of existing water hydraulic and quality modelling tools with their applications. Strategies for optimal control of DBPs are presented in Section 6. We conclude in Section 7.

2.0 FACTORS AFFECTING DBP FORMATION

Modelling the formation of DBPs necessitates the consideration of several influential parameters and governing equations within WDNs such as chlorine decay. While numerous studies have endeavored to explore some of these parameters to enhance the precision of water distribution system analysis and predictive models (Fisher et al., 2017; P. Hua et al., 2015; Mathieu et al., 2014; Tomlinson et al., 2016; Z. Wang et al., 2012, 2013), it remains the case that many controlling factors have not been fully characterized (K. Zhang et al., 2020).

2.1 Water quality

DBP formation is primarily influenced by several key factors including the disinfectant type and concentration, pH levels, the organic and inorganic composition of the water, as well as the water's temperature. A brief overview of the water quality factors affecting the DBP formation is presented in this section with a more detailed analysis found in deliverable D4.1.

Initially, as presented in Table 1, different DBPs are formed depending on the disinfection process which can include chlorine, chloramine, and chlorine dioxide use. Some water utilities use chloramines instead of chlorine as a final disinfectant to decrease the formation of C-DBPs such as trihalomethanes (THMs) and haloacetic acids (HAAs). However, if the source water is impacted by wastewater or algae, this could lead to an increase in the generation of halogenated N-DBPs such as haloacetamides (HacAms), halonitromethanes (HNMs), and haloacetonitriles (HANs) (H. Hong et al., 2023). In recent years, N-DBPs have attracted more attention due to their higher genotoxicity and cytotoxicity, despite their generally lower concentrations than currently regulated C-DBPs (S. Zhou et al., 2020). Among the new classes of N-DBPs, nitrosamines have recently been identified (Bond et al., 2011; Farré et al., 2011). These compounds are potent carcinogens, with nine types specified so far (Richardson & Plewa, 2020). Among them, N-nitrosodimethylamine (NDMA) has received the most research attention due to its high toxicity and detection rates especially in water reuse applications, focusing on its formation, occurrence, and control (Mitch et al., 2003). Using chloramine as a disinfectant may also result in the formation of other nitrosamines, such as N-nitrosodiethylamine (NDEA) (Liu et al., 2023). The presence of organic and inorganic components in water can impact the process of reducing chlorine dioxide, leading to the formation of the inorganic DBP chlorite, which can then convert into chlorate ions (Kurajica et al., 2020; Sathasivan et al., 2020).

The pH of water plays also a significant role in DBP formation. Increased pH levels tend to result in increased THM levels while causing the opposite effect on HAAs, as demonstrated in a study by Bond et al., (2012). Additionally, other groups of DBPs like HANs and haloketones (HKs) present instability at high pH levels, leading to their decomposition and subsequently promoting the formation of THMs and HAAs. Other studies have aimed to develop models to better understand these factors. These models assess the influence of pH on speciation coefficients, specifically in the context of bromide's impact on the formation of trihalomethanes and haloacetic acids (Roccaro et al., 2014).

Temperature also affects the rate of DBP formation. Generally, increased temperature leads to faster kinetics, thus faster DBP formation with different effects observed for specific DBPs. However, it's worth noting that volatilization serves as a mechanism for reducing DBP levels at relatively high temperatures, although this effect does not apply to non-volatile DBPs like HAAs. X. Zhang et al., (2013) investigated the effect of temperature in a suite of different DBPs. Within this study, the concentration of regulated DBPs such as chloroform, DCAA, and TCAA was found to increase with water temperature, while the typical emerging DBPs (DCAN, CH, TCNM1,1-DCPN, and 1,1,1-TCPN) displayed significant auto-decomposition, alongside initial concentration growth within the first few hours.

The precursors can be categorized as organic or inorganic and can further affect the DBP formation process. However, identifying these DBP precursors is a challenging task. Therefore, when modelling DBP formation, researchers often rely on bulk parameters such as total organic carbon (TOC) or total organic nitrogen (Krasner et al., 2009). In addition, both the quantity and composition of Natural Organic Matter (NOM) play significant roles in this process. NOM encompasses distinct types or categories, including allochthonous, which originates from terrestrial sources and is largely composed of humic substances, as well as autochthonous NOM, derived from microbial sources and characterized by a prevalence of non-humic organic matter. Additionally, algal organic matter and organic material from wastewater effluents further contribute to the complexity of DBP formation (Bond et al., 2012; Krasner, 2009).

In general, the studies that investigate the water quality parameters that affect DBP formation can be either focus on analyzing the reasons leading to chlorine decay (Curling et al., 2022; Nono et al., 2019; Powell et al., 2000; Vieira et al., 2004) or focus on the determinants of DBP formation itself (Brown et al., 2011a; P. Hua et al., 2015; Sohn et al., 2004).

2.2 Water network properties

Water hydraulic properties including water velocity, retention time in tanks, water age, and pipe material is another group of parameters proven to be affecting the rate of DBP formation (Lemus Pérez & Rodríguez Susa, 2017; Lemus-Pérez & Susa, 2020; H. Wang et al., 2017; Z. Wang et al., 2021; K. Zhang et al., 2020).

Extended residence time due to water stagnation can lead to the loss of disinfectant residual, reducing the ability to control microbial contaminants, and potentially allowing for bacterial regrowth. This, in turn, may alter the composition and concentration of DBPs in the water, as disinfectants like chlorine or chloramines interact with naturally occurring organic matter, leading to the formation of DBPs. Stagnant conditions can lead to higher DBP levels due to extended contact time between disinfectants and organic precursors (Abokifa et al., 2016b). Zhao et al., (2018), investigated the dependence of chlorine decay and DBP formation kinetics on pipe flow properties in drinking water distribution but only limited the study to THMs. In Abokifa et al., (2016a), the authors observed a significant impact of flow velocity on the formation of THMs from biomass, through two simultaneous processes. In the first one, the flow velocity improves the transfer of solutes across the interface of the bulk and biofilm, facilitating the movement of disinfectants and essential substrates. These factors are vital for regulating bacterial growth within the biofilm. In the second one, the increased flow velocity generates high shear stresses, which, in turn, lead to the detachment of biomass from the biofilm. Calculations using the Blasius equation demonstrate that shear stress increases nonlinearly with flow velocity under turbulent conditions. In another study, the role of biofilms in chlorinated WDNs is highlighted since their presence proved to cause a reduction of chlorine levels leading to the formation of significant quantities of harmful DBPs (J. Xu et al., 2018).

Pipe material and the corrosion rate within WDNs can further impact the removal of NOM and DBPs. Increased corrosion rates can lead to increased DBP removal, offering valuable insights for controlling these substances with various disinfection methods (H. Wang et al., 2017). In a recent study, the effect of copper ion (Cu^{2+}), a common corrosion product, on the degradation of trace pollutants was investigated in a Cu^{2+}/NH_2Cl system (Sheng et al., 2021). The study identified five DBPs, namely, trichloromethane (TCM), dichloroacetonitrile (DCAN), dichloroacetone (DCP), trichloronitromethane (TCNM), and trichloroacetone (TCP) during chloramination and their cytotoxicity and genotoxicity substantially increased when Cu^{2+} was present compared to chloramination without Cu^{2+}. Poleneni & Inniss, (2019) developed an array of predictive tools to better understand how wall effects affect the formation of DBPs in drinking WDN. To validate their findings on a WDN, they conducted various experiments examining materials, wall effects, bulk reactions, and water flow. Their research revealed a general increase in TTHM formation due to reactions on the pipe wall surfaces in PVC systems.

Further research is necessary to understand the physiochemical mechanisms underlying flow-dependent kinetics, such as biofilm-related wall demand, the role of material, and the age of pipes in a network. This is especially important for other families of DBPs, as it will help to determine how WDN conditions affect the rate of both disinfectant decay and DBP formation.

3.0 DBPs FORMATION PREDICTION THROUGH SENSING TECHNOLOGIES

3.1 UV-Vis Spectroscopy

The absorption of both visible and ultraviolet (UV) light by natural organic matter is mainly attributed to the presence of aromatic chromophores. When measuring and characterizing DBP precursors, certain surrogate parameters are widely used, including the absorbance of UV light at 254 nm (A_{254}) and the specific ultraviolet absorbance at 254 nm ($SUVA_{254}$), which is the ratio of A_{254} to DOC. SUVA254 is commonly used to compare different water sources in terms of their reactivity for DBP formation, typically measured as trihalomethane formation potential. However, it should be noted that SUVA254 measurements can be influenced by factors such as pH, nitrate, and iron, and there are ongoing discussions about its reliability as an indicator of DOC reactivity (Weishaar et al., 2003). Additionally, the absorbance at 280 nm is considered because it corresponds to the π-π* electron transition in the UV region (approximately 270-280 nm) for substances like phenolic compounds, aniline derivatives, benzoic acids, polyenes, and polycyclic aromatic hydrocarbons with multiple rings. Differential absorbance at wavelengths close to 272 nm (ΔA_{272}), which corresponds to the peak of differential absorbance, has been used due to its strong correlation with total organic halogen (TOX) levels and concentrations of individual DBPs during chlorination or chloramination (F. Zhang et al., 2022).

Reliable measurements were reported using the online UV-Vis instruments for water quality detection and water treatment process control. For example, various studies reported algorithms based on certain wavelengths (regions) of UV-Vis spectra to determine water quality, such as the use of absorbance ratios to monitor the variation of DOC in the water and multiple linear regression to estimate the total carbon contents in water (Barreto et al., 2004; Kim et al., 2016). Nonetheless, acquiring precise water quality measurements through online UV-Vis instruments equipped with integrated algorithms can pose difficulties, as they may suffer from under-compensation, over-compensation, and the inability to generate sensible measurements for real-time monitoring and process control (Y. Hu & Wang, 2017; Lepot et al., 2016).

Despite these limitations, online UV-Vis spectrophotometers are gaining popularity as preferred options for real-time monitoring and process control of water quality. The reason is that they offer several advantages, such as being reagent-free, eliminating the need for sample pre-treatments, and providing continuous measurements. These online UV-Vis sensors excel at capturing water quality events promptly and enabling faster responses to changes in water quality compared to traditional monitoring methods (Cheng et al., 2022). UV-Vis spectral detection has been introduced in many areas, including drinking water quality, disinfectant residual, and disinfection by-product formation (Hou et al., 2014; Roccaro et al., 2015).

3.2 Fluorescence Spectroscopy

Fluorescence spectroscopy is a non-invasive and sensitive technique that allows the analysis of DOM based on its fluorescence properties by scanning a range of excitation and emission wavelengths. Fluorescence technology for DOM characterization has several advantages: it is rapid, sensitive, and requires minimal sample preparation. Additionally, it allows for real-time monitoring and can be applied in situ, enabling continuous measurements in natural water systems. Due to its simplicity of usage can be employed as a sensor and help in understanding the formation, transformation, and fate of DBP formation in different water sources and treatment processes.

Bridgeman et al., (2011) reviewed the applications of fluorescence techniques to DOM characterizations with a focus mostly on the disinfection process and DBP formation. A substantial body of literature has now established connections between fluorescence spectra and the physicochemical properties of DOM (L. Li et al., 2020).

More importantly, researchers have utilized fluorescence spectroscopy to characterize the alterations in DOM following disinfection and have explored the association between fluorescence properties and the formation of DBPs (Korshin et al., 1999; Roccaro et al., 2009; Westerhoff et al., 1999). L. Yang, Hur, et al., (2015) provide a summary of correlations established using the linear regression method for DBPs derived from partial carbon sources. They explore various fluorescence parameters such as fluorescence intensity, intensity ratios, fluorescence region integrals, and other relevant parameters, aiming to develop models for fitting purposes. Peleato et al., (2018) proposed autoencoder-neural network regression to predict the formation of DBPs. Investigations extend beyond carbon-containing disinfection byproducts to also include nitrogen-containing disinfection byproducts. However, it has been observed that correlations between N-DBPs and fluorescence indices are generally weaker compared to the correlations between C-DBPs and fluorescence indices (Ma et al., 2016). Nevertheless, the utilization of fluorescence techniques for monitoring drinking water treatment encounters several challenges. One of these challenges is the inherent variability in water quality among different sources, leading to significant variations in the composition of DOM despite the presence of similar fluorescence levels on fluorescence maps.

Consequently, this diversity in DOM composition gives rise to a multitude of correlations, thereby complicating the interpretation and practical application of fluorescence techniques in the context of drinking water monitoring. Another limitation in the application of fluorescence techniques for drinking water treatment monitoring is the predominant emphasis on the direct utilization of excitation/emission (Ex/Em) pairs and fluorescence intensity by current fluorescence sensors. These parameters, while relatively simple, have certain drawbacks as highlighted by Wasswa et al., (2019), particularly when background fluorescence is noisy, leading to the omission of valuable information. To address this issue, there is an urgent need for the development of sensors that can extract more comprehensive information and integrate mathematical algorithms into the monitoring system. Considering that EEMs

are intricate maps, the integration of image recognition technology, which can effectively extract key features and analyze intricate details, holds the potential to overcome these limitations (L. Li et al., 2020).

3.3 Biosensors

A biosensor is a device that has a biological recognition element that is intricately embedded and serves as the primary discriminating factor (whether physically connected or enclosed) (Kissinger, 2005). The type of bio-chemical process occurring within the fixed layer and the intended use of the biosensor influence the choice of the biological recognition element (Smutok & Katz, 2023). The same (bio)chemical process that detects the presence of the analyte can be implemented using a variety of physical transduction techniques, including thermal, piezoelectric, optical, and electrochemical (Rodriguez-Mozaz et al., 2005). Nevertheless, these devices are more used to detect DBPs than DBP precursors.

Electrochemical biosensing has emerged as a promising alternative for monitoring DBPs in water sources due to its ability to offer rapid, affordable, and sensitive detection, in contrast to conventional laboratory techniques. W. Zhang et al., (2019) recently reviewed the state-of-the-art electrochemical sensors and listed the developed sensors that have mostly been used to detect trichloroacetic acid (TCA). Nevertheless, the main limitation is still related to the long-term storage difficulties of the immobilized biological recognition molecules. In this sense, molecular imprinted polymers (MIPs) are attracting increasing attention due to their low production cost, long shelf-life, reusability without loss of selectivity, ease of preparation, high mechanical strength, and high thermal and chemical stability (Cetó et al., 2016; Kibechu et al., 2014).

Other methods have been developed to measure DBPs online, such as sensors based on the Fujiwara reaction (Lugg, 1959).

4.0 DBP MODELLING

Different mathematical models have been proposed to understand and predict DBP formation. Modelling can serve various purposes, such as identifying the crucial operational and water quality parameters that control the formation of DBPs or studying the kinetics involved in their formation (Premarathna et al., 2023; Zhao et al., 2018). Additionally, some models are designed to predict DBP formation as an alternative to field monitoring (Ata et al., 2015).

To create predictive models for DBPs, it is necessary to establish both empirical and mechanistic relationships between water quality and operational parameters and the levels of DBPs present at different stages after water treatment (Sadiq & Rodriguez, 2004). The categorization of mathematical models is based on whether their formulations are grounded solely on empirical/statistical foundations or whether they

stem from mechanistic principles based on idealized functional characteristics or behaviours (Ike et al., 2020).

In Figure 1, the DBP predictive models are categorized based on various classification criteria. The categorization can be based on the method, the tool or the variables utilized for estimating the DBP formation and concentration.

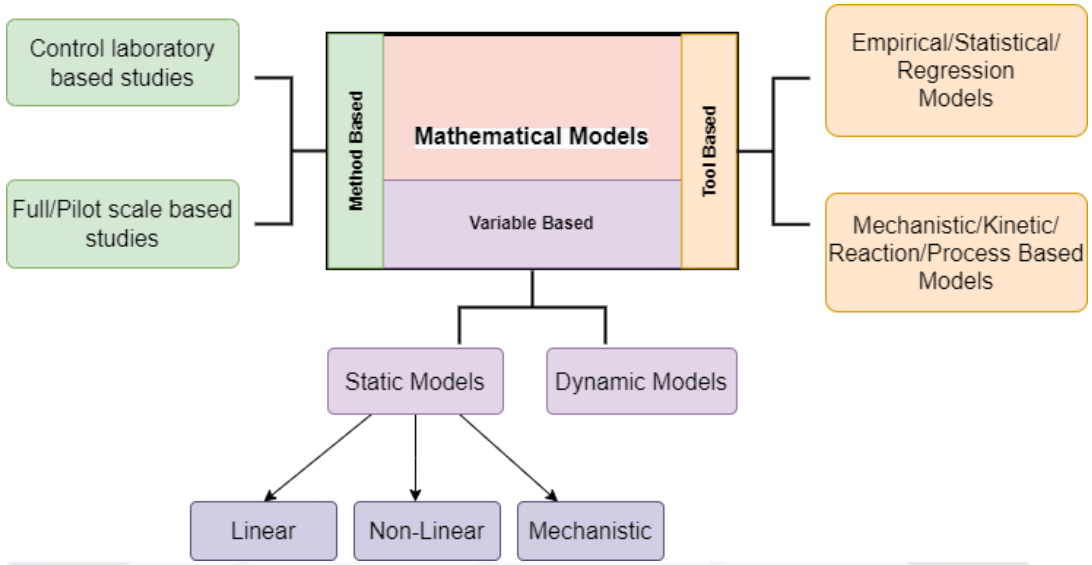


Figure 1: Categorization of DBP models

In a review by Sadiq & Rodriguez, (2004), mathematical models, published from 1983 to 2003, utilized for estimating both inorganic and organic DBPs using only static variables were examined, whereas Beauchamp, Dorea, et al., (2018) recently conducted a review study focusing on dynamic variable models that utilized differential absorbance to estimate the concentrations of DBPs.

Empirical models, also known as statistical models or regression models, describe the relationship between the concentrations of disinfectants, precursors, and other water quality parameters and the concentrations of DBPs. They typically use statistical methods such as regression analysis to identify the most significant predictors of DBP formation and to develop predictive equations. These models are often used when there is limited information on the chemistry of DBP formation (Bond et al., 2014; Chowdhury et al., 2009; Sadiq & Rodriguez, 2004). Most studies use Multiple Linear Regression (MLR) models to predict different DBPs (Ata et al., 2015; Babaei et al., 2015; Beauchamp et al., 2019; Domínguez-Tello et al., 2017; H. C. Hong et al., 2007; J. Lin et al., 2018; Obolensky & Singer, 2008; Shahi et al., 2020; Uyak et al., 2007; Valenti-Quiroga et al., 2022), with other types of regression models used, as well, such as Robust Poisson Regression (Font-Ribera et al., 2017), log-log linear regression (Mouly et al., 2010), multivariate regression equations (Rodriguez et al., 2004) and a combination between several regression models (Trueman et al., 2016). Other studies considered the use of regression models with neural networks (NN) (H. Lin et al., 2020; Mian et al., 2021; Z. Xu et al., 2022) and genetic algorithms (GA) (Liu et al., 2023).

Mechanistic models, also known as kinetic models, reaction models, or process-based models, describe the underlying chemical and physical processes that govern the formation and transformation of DBPs. They typically use rate and mass balance equations to quantify the kinetics of individual reactions and the overall formation of DBPs. Mechanistic models can be more accurate but require more information regarding the chemistry and the kinetics of DBP formation (Chowdhury et al., 2009; Sadiq & Rodriguez, 2004). In Gang et al., (2002), the authors developed a simple mechanistic model to predict TTHM and the sum of nine haloacetic acids (HAA9) formation based on chlorine demand. A variable reaction rate model was also proposed by (P. Hua et al., 2015). In this study, a second-order kinetic model was proposed for simulating chlorine decay in bulk water considering the reaction with dissolved organic matter (DOM).

According to the characteristics of the input variables, models are classified into two categories: static variable models (SV) and dynamic variable/differential models (DV). SV models use static variables as inputs, except for the time parameter, while DV models rely on dynamic variables that are altered due to disinfection (Ike et al., 2020). It has been observed that the differential parameters in DV models serve as generic compact sub-models that function as local time parameters, representing the destruction of UV or fluorescence excitation-emission matrices (FEEM) or chlorine decay. However, these parameters do not precisely track the so-called DBP chromophores, as mentioned in the previous study. Further, a model based on the concept of electron delocalization (ED) was proposed to explain the unique photophysical properties of dissolved organic matter (DOM) following chlorination, chloramination and other common physical and chemical treatments. A comprehensive and consistent explanation of DOM's photophysics is further presented.

A systematic review of models employed for DBP formation published from 1983 up to today has been conducted. The most cited 105 models were identified and divided into static variable models (Table 2, Table 3 and Table 4) and dynamic variable models (Table 5).

4.1 DBP Static Model

There are various methods for estimating DBPs in drinking water, and the choice of method will depend on the specific type of DBP and the available resources. This section presents various types of modelling methods used for DBPs modelling, including Regression, Machine Learning, Fuzzy Logic, Mechanistic, etc.

4.1.1 Regression methods

Statistical models produce regressions relating DBP concentrations to known reaction conditions at the beginning of the disinfection process (e.g., initial NOM and Cl_2 concentrations, temperature, pH, etc). Such models often use the chlorine concentration in the original solution (i.e., based on the Cl_2 dose) to characterize the system throughout the reaction period, even though that concentration might change dramatically during the reaction (Korshin et al., 2004). The produced linear or multiple

regressions aim to derive from a dataset a linear relationship between the independent variable X_i and the dependent variable Y_i that minimizes the distance (or error) between the line and the data points. Regression is used to predict or estimate an output value based on one or more input values. In the case of the multiple regression method applied to DBPs, the equation can be written as:

$$DBP_s = \beta_0 + \sum_{1}^{p} \beta_i X_i + \varepsilon_i$$

where β_0 is the intercept, X_i is the independent variable and ε the error (Stock et al., 2005). The independent variable (X_i) is generally the measurement of water quality indicators, and other parameters that characterize the disinfection process such as t, Cl_2, Br^-.

As shown in Table 2, regression methods are largely the most used in studies dealing with DBPs modelling. They use empirical data obtained in the laboratory or in the field (pilot or full scale) to predict the concentration of DBPs in specific operating conditions. Even though such models are not theoretically based, they use many parameters that are known to affect DBPs formation. The most used water quality parameters in DBPs regression models are reaction time (t), temperature (T), bromide concentration (Br^-), disinfectant concentration (e.g., Cl_2), pH, DOC, TOC, UV_{254}, and in some cases fluorescence indexes (Table 2). Disinfectant dose and reaction time are the main drivers for the formation of DBPs. Furthermore, T is a fundamental parameter that strongly impacts the DBPs kinetic formation, Br^- is a relevant inorganic precursor in DBP formation and affects the speciation of many DBPs (e.g., the higher the Br^-, the higher the concentration of the brominated organic by-products is). The DOC/TOC, UV_{254}, and fluorescence indexes, are indicators of organic precursors because they measure the content of NOM that can react with chlorine to form DBPs. Indeed, since NOM is a complex entity, whose reactive sites are unknown, measurements of bulk organic content (DOC/TOC), chromophores, and fluorophore in NOM are used as surrogates of NOM content and reactivity in DBP formation. Finally, pH is often employed in regression models because can impact the formation mechanism. For instance, the formation of a specific DBP may be inhibited or enhanced at varying pH because the mechanisms that cause the release of some individual DBP (e.g., THMs) from their precursors include hydrolysis. Regarding the class of DBPs investigated, THMs and HAAs are the main classes of DBPs modelled, even though some model is focused on HNMs (Guilherme & Rodriguez, 2017), HANs, HKs (Guilherme & Rodriguez, 2017), HAcAms (Chu et al., 2012), NDMA (L. Yang, Kim, et al., 2015), chlorite (Korn et al., 2002), and bromate (Song et al., 1996; Tyrovola & Diamadopoulos, 2005). A large number of models are developed based on laboratory data, although the use of full-scale data for DBPs modelling has increased. Finally, a massive number of regression models are based on raw water because of the high concentration of precursors, while much fewer models are focused on treated/tap waters. Synthetic waters are also used to simulate the NOM content in water.

Table 2: Empirical models with static variables

Type of water	DBP modelled (output)	Input parameters	Type of model	Scale	Reference
Raw water and treated water	THMs	Br^-, Cl_2, pH, T, NVTOC	Multiple regression	Lab scale and Full scale	(Morrow & Minear, 1987)
Raw water	THMs	Br^-, Cl_2, pH, T, NVTOC	Multiple regression	Lab scale	(Minear & Morrow, 1983)
Raw water	THMs	Br^-, Cl_2, pH, t, T, TOC, UV_{254}	Multiple regression	Lab scale	(Amy et al., 1987)
Raw water	$CHBr_3$, TOBr, Bromate	Br^-, pH, t, T, DOC, O_3	Multiple regression	Lab scale	(Siddiqui & Amy, 1994)
Raw water	Bromate	Br^-, pH, t, DOC, O_3, NH_3-N, IC	Multiple regression	Lab scale	(Song et al., 1996)
Raw water	$CHCl_3$, BDCM, DBCM, $CHBr_3$	Br^-, Cl_2, pH, DOC	Multiple regression	Lab scale	(Rathbun, 1996b)
Raw water	THMs	Cl_2, t, TOC, UV_{254}	Multiple regression	Lab scale	(Chang et al., 1996)
Raw water	THMs. NPTOX	Cl_2, pH, t, UV_{254}	Multiple regression	Lab scale	(Rathbun, 1996a)
Raw water	THMs	Br^-, Cl_2, pH, t, T, DOC	Multiple regression	Lab scale	(Amy, 1998)
Raw water	ClO^-_2	Cl_2, t, T, TOC, UV_{254}, ClO_2, NPOC	Multiple regression	Lab scale	(Korn et al., 2002)
Raw water	THMs	Cl_2, pH, t	Multiple regression	Lab scale	(Nikolaou et al., 2004)
Raw water	THMs, DCAN, TCP	Cl_2, pH, t, TOC	Multiple regression	Lab scale	(Boyalla, 2004)
Raw water	THMs, HAA	Br^-, Cl_2, pH, t	Multiple regression	Lab scale	(Lekkas & Nikolaou, 2004)

Raw water	Bromate	Br^-, pH, t, O_3	Multiple regression	Lab scale	(Tyrovola & Diamadopoulos, 2005)
Raw water	THMs	Br^-, Cl_2, pH, t, TOC	Multiple regression	Lab scale	(Al-Omari et al., 2005)
Raw water	THMs, $CHCl_3$, BDCM	Br^-, Cl_2, pH, t, T, DOC	Multiple regression	Lab scale	(H. C. Hong et al., 2007)
Raw water	THMs, HAA	Br^-, Cl_2, t, T, pH, DOC, UV_{254}	Multiple regression	Lab scale	(H. C. Hong et al., 2008)
Raw water	THMs-Br	Br^-, t, pH, DOC, NH_3-N	Multiple regression	Lab scale	(Wang et al., 2010)
Raw water	THMs	Br^-, Cl_2, T, TOC, UV_{254}	Multiple regression	Lab scale	(Brown et al., 2011b)
Raw water	THM_4. HAA_9	Br^-, Cl_2, DOC	Multiple regression	Lab scale	(Bond et al., 2014)
Raw water	THMs	T, pH, DOC	Multiple regression	Lab scale	(G. feng Yang et al., 2014)
Raw water	THMs, HAA9	Cl_2, Model costant, NOM	Multiple regression	Lab scale	(Peleato & Andrews, 2015)
Raw water	THMs	Model costant, DOC, UV_{254}	Multiple regression	Lab scale	(Awad et al., 2016)
Raw water	THMs, HANs	Br^-, Cl_2, t, T, pH, DOC	Multiple regression	Lab scale	(H. Hong et al., 2016)
Raw water	THMs, HAA	Br^-, Cl_2, t, T, DOC, UV_{254}, UV_{272}	Multiple regression	Lab scale	(Alver et al., 2018)
Raw water	THMs, HAA5	Cl_2, t, TOC, UV_{254}	Multiple regression	Lab scale	(Roth & Cornwell, 2018)
Raw water	THMs, HAAs, HANs	Br^-, Cl_2, t, T, pH, DOC, UV_{254}	Multiple regression	Lab scale	(J. Lin et al., 2018)
Raw water	THMs, HAA	DOC, UVA_{254}	Linear regression	Lab scale	(Milstead & Remucal, 2021)

Raw water and synthetic water	DCAcAm	Br^-, DOC, AP ,DON , SMP	Multiple regression	Lab scale	(Chu et al., 2012)
Raw water and treated water	THMs, HAA6, TOBr	Br^-, Cl_2, pH, t, T, DOC, UV_{254}, H_2O_2, O_3, NH_3–N	Multiple regression	Lab scale	(Sohn et al., 2004)
Raw water and treated water	THMs, NDMA	DOC, Bromide, UV_{254}, EEM humil-like an tryptolphan like componentes	Linear regression	Lab scale	(L. Yang, Kim, et al., 2015)
Synthetic water	$CHCl_3$	Cl_2, TOCD, t, k (reaction rate)	Multiple regression	Lab scale	(Engerholm & Amy, 1983)
Synthetic water	THMs	Cl_2, pH, TOC, t, k (reaction rate), m and n (model constant)	Multiple regression	Lab scale	(Urano et al., 1983)
Synthetic water	THMs	Br^-, Cl_2, pH, t, T, TOC, UV_{254}	Multiple regression	Lab scale	Harrington G.W. et al (1992)
Synthetic water	POX, NPOX	Cl_2, pH, t, T, TOC	Multiple regression	Lab scale	(Huixian et al., 1997)
Synthetic water	BDCM	Br^-, Cl_2, t, T, pH, DOC	Multiple regression	Lab scale	(Chowdhury, Champagne, & James McLellan, 2010)
Synthetic water	THMs	Cl_2, t, T, pH, DOC	Multiple regression	Lab scale	(Chowdhury, Champagne, & McLellan, 2010)
Synthetic water	TOBr, THMs	Br^-, Cl_2, t, ph, DOC, NH_3-N, O_3	Multiple regression	Lab scale	(T. Lin et al., 2014)
Treated water	THMs, HAA	Cl_2, t, T, TOC	Multiple regression	Lab scale	(Sérodes et al., 2003)
Treated water	THMs, $CHCl_3$, BDCM, DBCM, $CHBr_3$	Cl_2, T, FA	Multiple regression	Lab scale	(Rodrigues et al., 2007)
Treated water	THMs	Cl_2, t, BOD	Multiple regression	Lab scale	(Haddad et al., 2014)

Raw water and treated water	THMs	Br^-, Cl_2, t, UV_{254}	Multiple regression	Full scale and Pilot scale	(Semerjian et al., 2009)
Ballast water	DBCM, TBM	Cl_2, t, T, pH, Sal, DO, Chl, Tur	Multiple regression	Full scale	(X. Zhang et al., 2019)
Raw water	$CHCl_3$	pH, T, δ, ε (error)	Multiple regression	Full scale	(Garcia-Villanova, Garcia, Alfonso Gomez, et al., 1997)
Raw water	THMs	Br^-, Cl_2, pH, T, Chla, S and Sp	Multiple regression	Full scale	(Golfinopoulos et al., 1998)
Raw water	THMs	Cl_2, pH, t, T, DOC	Multiple regression	Full scale	(Rodriguez et al., 2000)
Raw water	THMs	Br^-, Cl_2, pH, t, T, DOC	Multiple regression	Full scale	(Westerhoff et al., 2000)
Raw water and treated water	$CHCl_3$	Cl_2, pH, T, Fluorescence	Multiple regression	Full scale	(Ibarluzea et al., 1994)
Raw water and treated water	THMs, $CHCl_3$, BDCM	Br^-, Cl_2, pH, T, Chla, S, Sp	Multiple regression	Full scale	(Golfinopoulos & Arhonditsis, 2002)
Raw water and treated water	THMs	Cl_2, pH, T, TOC	Multiple regression	Full scale	(Uyak et al., 2005)
Raw water and treated water	THMs	Cl_2, T, TOC	Multiple regression	Full scale	(Toroz & Uyak, 2005)
Raw water and treated water	HAAs	Br^-, Cl_2, t, T, TOC, UV_{254}	Multiple regression	Full scale	(Y. Zhang et al., 2011)
Raw water and treated water	THMs	Cl_2, t, T, pH, UV_{254}	Multiple regression	Full scale	(Kumari & Gupta, 2015)
Raw water and treated water	THMs	Br^-, Cl_2, t, T, Seasons	Linear regression	Full scale	(Ramavandi et al., 2015)
Raw water and treated water	THMs	Br^-, Cl_2, t, T, pH, DOC, UV_{254}	Multiple regression	Full scale	
Raw water and treated water	THMs	Cl_2, T, DOC	Multiple regression	Full scale	(Valdivia-Garcia et al., 2016)

Raw water and treated water	THMs	Cl_2, t, T, pH, TOC	Data analyst	Full scale	(Saidan et al., 2016)
Raw water and treated water	THMs	Br^-, Cl_2, t, T, pH, DOC, UV_{254}	Multiple regression	Full scale	(Domínguez-Tello et al., 2017)
Raw water and treated water	THMs, HAAs, HNMs, HANs, HKs	Cl_2, T, pH, DOC, UV_{254}, Tur	Multiple regression	Full scale	(Guilherme & Rodriguez, 2017)
Raw water and treated water	THMs, HAA	Br^-, Cl_2, t, T, DOC, UV_{254}, DON, FI	Multiple regression	Full scale	(Chowdhury, 2018)
Raw water and treated water	THMs, HAA	Br^-, Cl_2, t, T, pH, DOC, UV_{254}	Multiple regression	Full scale	(Shahi et al., 2020)
Raw water and treated water	THMs	Br^-, Cl_2, t, T, TOC, UV_{254}	Multiple regression	Full scale	(Godo-Pla, Emiliano, et al., 2021)
Raw water, treated water and tap water	TTHM	Cl_2, t, T, pH, TOC, Tur, TS, Alk, EC	Multiple regression	Full scale	(Salam Hussein et al., 2020)
Treated water	$CHCl_3$	pH, T, Y, ε (error)	Multiple regression	Full scale	(Garcia-Villanova, Garcia, Gomez, et al., 1997)

4.1.2 Mechanistic approach

Mechanistic models are based on physical or phenomenological parameters that are consistent with the fundamental theory of the original complex processes (Ike et al., 2020). They often incorporate *a priori* assumptions of first- or second-order kinetics, so that the integrated rate equations have forms similar to those shown for chlorine consumption. For instance, in some cases, the yield of individual DBPs has been modelled as being linearly proportional to the chlorine consumption. Another key element in any fundamentally sound model is the recognition of the step-wise incorporation reactions of chlorine, leading to the formation of intermediates from which individual DBPs are released (Korshin et al., 2004). Recently, various models have been based on the assumption that NOM molecules have two or more kinetically distinct sites for reactions with chlorine that result in different short- and long-term DBPs formations (Korshin et al., 2004; Roccaro et al., 2013). Such models can be calibrated and validated also using statistically derived kinetic parameters such as reaction rate constants. Mechanistic models are used not only for predicting the concentration of DBPs but also the DBPs speciation (Nokes et al., 1999; Roccaro et al., 2013). In the latter case, it is often assumed that the halogenated precursors are formed by successive steps, each of which substitutes either bromine or chlorine into an activated site in the NOM (Yan et al., 2016).

As shown in Table 3, the number of papers on mechanistic models is much lower than that dealing with statistical models. In most cases, the used data are obtained by laboratory experiments exploring the kinetic of THMs or HAAs formation. A few models also investigate the formation of other DBPs, such as HANs (Roccaro et al., 2013) or HNMs (Zhu & Zhang, 2016). The most used type of water is raw water which has a higher precursor content and results in higher DBPs concentration. Some mechanistic models reported in Table 3 are speciation models (Nokes et al., 1999) that can predict the speciation of chlorinated, brominated, and in a few cases iodinated DBPs (Yan et al., 2016). Recently, the combination of experimental and quantum-chemical data has been successfully used to model the formation and speciation of THMs and HAAs during chlorination or chloramination (C. Zhang et al., 2020).

Table 3: Mechanistic models with static variables

Type of water	DBP modelled (output)	Input parameters	Type of model	Scale	Reference
Raw water	THMs, HAAs	Developed several models as a function of various reaction coefficients	Probabilistic model	Lab scale	(Uyak & Toroz, 2007)
Raw water	Iodine-, Bromine- and Chlorine- THMs	Bromine and iodine incorporation coefficient	Ternary halogenation modeling	Lab scale	(Yan et al., 2016)
Raw water	THMs, HAAs	Rate constant	Quantum chemical and differential absorbance	Lab scale	(C. Zhang et al., 2020)
Raw water and synthetic water	THMs	Cl_2, K_1,K_2 K_3 model costant, t, TOC	Kinetic model	Lab scale	(Adin et al., 1991)
Raw water and synthetic water	THMs	Ca ([Cl_2]), pH, t, T, K (model constant), CAo, TOC	Kinetic model	Lab scale	(Clark & Sivaganesan, 1998)
Raw water and synthetic water	THMs	Br^-, Cl_2, pH, t, K, u e M (Costant model)	Kinetic model	Lab scale	(Clark et al., 2001)
Raw water and treated water	THMs, HAAs	Developed several models as a function of various reaction coefficients	Kinetic model	Lab scale	(Gang. Et al., 2002
Raw water and treated water	TDHAN	Br-, Cl_2, t, T, pH, $SUVA_{254}$, Rate constant	Kinetic model	Lab scale	(Roccaro et al., 2013)
Raw water and treated water	THMs, HAAs	Bromine incorporation coefficient	Modelling of dimensionless ratios	Lab scale	(Roccaro et al., 2014)
Synthetic water	TOX (TOCl, TOBr, TOI)	Developed several models as a function of various reaction coefficients	Kinetic model	Lab scale	(Zhu & Zhang, 2016)
Synthetic water	HNMs	Model constant	Kinetic model	Lab scale	(Xie et al., 2017)
Treated water	THMs	Developed several models as a function of various reaction coefficients	Kinetic model	Lab scale	(Nokes et al., 1999)
Raw water	THMs	Model constant	Kinetic model	Full scale	(Di Cristo et al., 2015)

Raw water and treated water	THMs, HAAs	Consumated chlorine	Kinetic model	Full scale	(Sathasivan et al., 2020)
Treated water	THMs	Developed several models as a function of various reaction coefficients	Kinetic model	Full scale	(Elshorbagy et al., 2000)
Treated water	THMs	Cl_2, pH, t, NVTOC	Kinetic model	Full scale	(Lou & Chiang, 2009)

4.1.3 Artificial intelligence and Machine Learning

Machine Learning (ML) is a subset of Artificial Intelligence, and in general, focuses on developing algorithms and models that allow computers to learn from data and make predictions or decisions based on this learning. ML is widely used in a wide range of applications, including prediction, classification, clustering, pattern recognition, and optimization. Due to these capabilities, in recent years it has been widely used in various fields, among these, as a model for predicting the presence of DBPs in drinking water (Table 4).

Computational intelligence (CI) is another subset of Artificial Intelligence, focusing on nature-inspired computational paradigms. One type of a CI model is the artificial neural network (ANN), a learning model inspired by the functioning of biological neurons and designed to learn from data by processing information in layers of artificial neurons. Another model is described by Fuzzy Logic (FL), which is used to imitate human reasoning and cognition. Rather than considering binary cases of truth, fuzzy logic includes 0 and 1 as extreme cases of truth but with various intermediate degrees of truth. Therefore, fuzzy logic is a mathematical theory and approach to information processing that differs from traditional classical binary logic, which assigns strictly true or false values (1 or 0) to every statement. Fuzzy Logic, assigns partial truth values, defined by a continuous set of possibilities between 0 and 1. This type of logic is particularly useful when it comes to representing human reasoning, where we often encounter nuanced, ambiguous, or uncertain situations. The key concept in fuzzy logic is that of "membership function". A membership function associates each element of a set with a value in the range [0, 1], indicating to what extent the element belongs to the set. For example, we can define a "high" set with a membership function that assigns high values (close to 1) to heights above a certain threshold and low values (close to 0) to heights below that threshold. In this way, it is possible to represent the gradient of different heights (Hájek, 1998; Kosko, 1997). As shown in Table 4, fuzzy logic has been also used to model DBPs formation at both lab and full scale (Godo-Pla, Rodríguez, et al., 2021; J. Zhang et al., 2023).

Machine learning algorithms can be used in symbiosis with mathematical models to obtain more accurate results, for example, the use of fuzzy logic in RBF (Radial Basis Functions) neural networks (J. Zhang et al., 2023).

Table 4: AI models with static variables

Type of water	DBP modelled (output)	Input parameters	Type of model	Scale	Reference
Raw water and treated water	DCAN, CPK, TCP	Cl_2, T,pH, DOC, UV_{254}, Tur, EC	LRM, Classification trees and ANN	Full scale	(G. Hu et al., 2023)
Tap water	HAA	Br^-, Cl_2, t, T, pH, DOC, UV_{254}, [NO_2^-] e [NH_4^+]	LRM, RBF ANN	Full scale	(H. Hong et al., 2020)
Tap water	HAA	Br^-, Cl_2, t, T, pH, DOC, UV_{254}, [NO_2^-] e ammonia[NH_4^+]	LRM, RBF ANN	Full scale	(H. Lin et al., 2020)
Tap water	HKs	pH, DOC, UV_{254}	Linear regression	Lab scale	(Deng et al., 2021)
Raw water and treated water	THMs	Br-, DOC, UV_{254}, C_1, C_2, C_3, Fmax	Classification trees	Full scale	(Bergman et al., 2016)
Raw water and treated water	THMs	t, T, pH, TOC, Tur, EC	Fuzzy logic	Full scale	(Godo-Pla, Rodríguez, et al., 2021)
Tap water	THMs	Cl_2, t, T, pH, UV_{254}	LRM, RBF ANN	Lab scale	(Z. Xu et al., 2022)
Tap water	THMs	T, DOC, NO_2^-, THMs	RBF ANN, Fuzzy logic	Lab scale	(J. Zhang et al., 2023)
Raw water	THMs, $CHCl_3$, $CHCl_2Br$, $CHBr_2Cl$, $CHBr_3$	Br^-, Cl_2, t, T, pH, DOC	ANN, SVM e GEP	Lab scale	(Singh & Gupta, 2012)
Raw water and treated water	THMs, HAAs	EEM humic-like componentes	PCA and PARAFAC and ANN Autoencoder	Pilot scale	(Peleato et al., 2018)
Synthetic water	TOX	Br-, Cl_2, NOM	LRM, RBF and BP ANN, SVM	Lab scale	(Bu et al., 2023)
Raw water and treated water	TOX, HAA, THMs	Br^-, Cl_2, pH, t, T, TOC, UV_{254}	ANN BP	Lab scale, Pilot scale and Full scale	(Kulkarni & Chellam, 2010)

4.1.4 Method Comparison

Among the SV models, many empirical models are available, while the number of mechanistic models is much lower (Figure 2). This result is probably because the empirical models are often based on simple statistic/regression analysis that does not require a deep understanding of the phenomenon. Therefore, empirical models are site-specific and cannot be easily applied to other cases. On the other hand, mechanistic models require an *a priori* definition of the model based on the formation mechanism theory. Such models can be calibrated and validated by using different water quality and operating conditions. Although it is thought that mechanistic models do not substantially improve the accuracy of DBPs prediction (Ike et al., 2020), it is clear that such models can also help to better understand the DBPs formation mechanism. A subset of SV models based on AI are emerging and the related number of published papers seems to follow an exponential increase rather than a linear one observed for both empirical and mechanistic models. As a result, in the future it is expected a relevant contribution of AI-based models on the modelling and monitoring of DBPs formation.

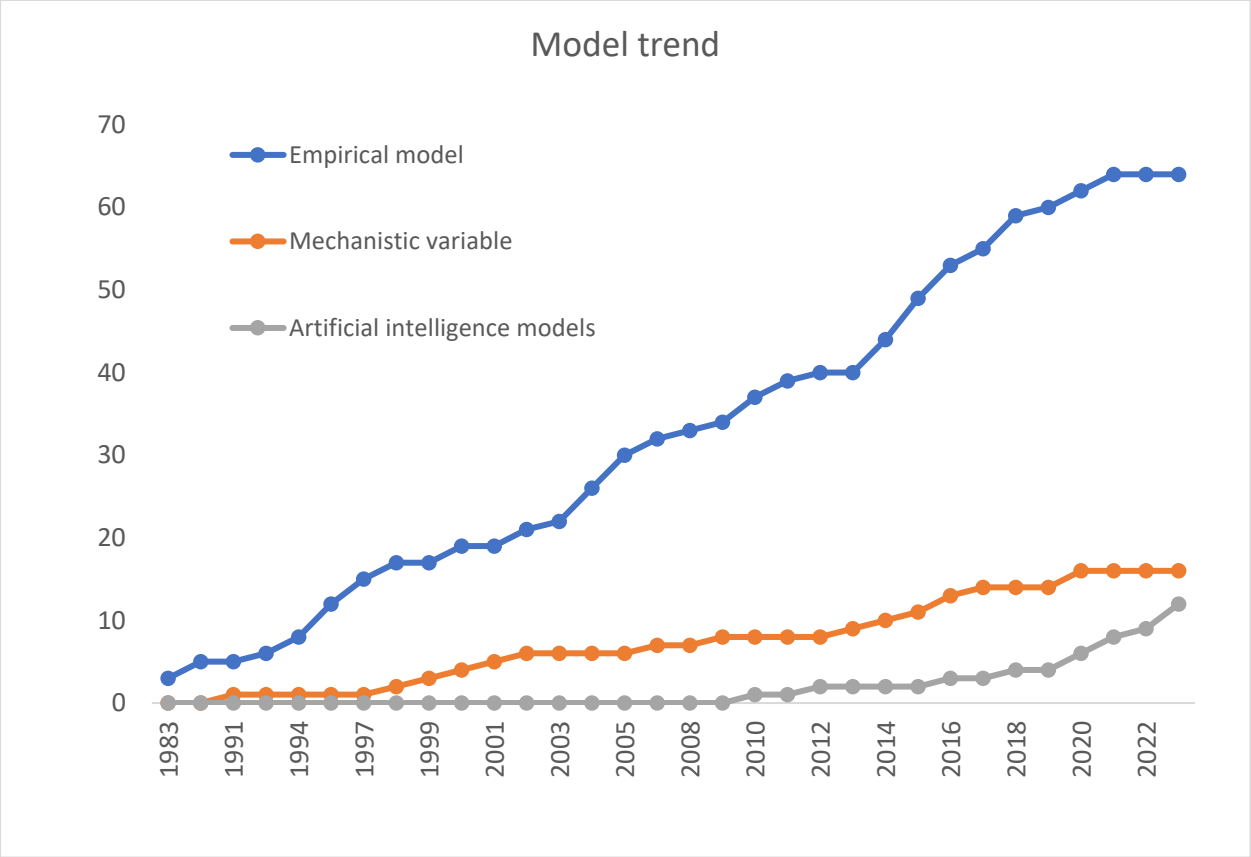


Figure 2: Cumulative sum of published papers on empirical, mechanistic and AI-based models.

4.1.5 Gaps and critical analysis

From the review of literature on SV models the following gaps and critical analysis can be summarized:

- Many studies are carried out in a laboratory using synthetic waters or raw waters, while the use of treated/tap waters is limited. This is relevant because tap water has a concentration of precursors lower than raw water. Therefore, modelling drinking water (i.e., treated/tap water) in distribution systems can be much more challenging.
- In some cases, the synthetic organic matter is not representative of the real NOM. Such papers are not reported in this review.
- Many models output refers to specific classes of DBPs, mainly THM and HAA, while other ubiquitous DBPs are scantily reported.
- Many models' outputs are the sum of specific classes of DBPs, while the speciation models are limited. This is not relevant for compliance to regulation but it is important from a scientific perspective. For instance, the brominated and iodinated organic DBPs are more toxic than their chlorinated analogues.
- The number of mechanistic models is much lower than statistical models. However, the latter are often not very useful understanding the phenomenon, while mechanistic models can gather more useful information that can help building a more general model. Furthermore, the use of quantum chemistry and/or AI coupled with the mechanistic/deterministic models can lead to important improvement in understanding the DBPs formation and fate in water.
- DBPs models applied to real water networks are very limited and there is a relevant gap to be covered in this area.

4.2 DBP Dynamic Model

In this section, we explore and present various types of DV models used for estimating DBP concentration in WDN. As aforementioned, DV models establish relationships between DBPs and specific alterations in water properties resulting from the chlorination or chloramination process. These changes, though capable of directly estimating DBP concentrations, are typically expressed differentially. This means they are presented as the variance between the initial value of the target parameter and its subsequent values over time as chlorination or chloramination proceeds.

In Table 5 we present various chemical models utilized for the prediction of the formation of DBPs, along with their corresponding kinetic parameters. The table offers insights into the different chemical reactions that contribute to the formation of DBPs, such as THMs, HAAs, chlorite, and chlorate. Each chemical model is linked to specific kinetic parameters, including rate constants and reaction orders, which are critical in predicting the DBP concentrations under different disinfection conditions. Additionally, Table 5 includes information regarding the disinfectants and precursors involved in these reactions, as their involvement plays a significant role in the formation and

speciation of DBPs. By understanding the kinetics of these chemical reactions, water utility managers and researchers can develop strategies to minimize DBP formation while maintaining effective disinfection.

Further, absorbance and fluorescence dynamic models have been developed for estimating the formation of DBPS. However, these models were mainly focussed on raw and treated water with limited applications on WDN. An overview of these modelling approaches is presented in Table 6.

Overall, this comprehensive compilation of chemical models and their kinetic parameters expands our understanding of the complex reactions governing DBP formation and contributes to the development of robust and sustainable water treatment practices.

4.2.1 Kinetics of DBP — Chemical reactions

To optimize chlorine dosage, minimize DBP formation, and strategically plan booster chlorinations within WDNs, we need a precise and universally applicable kinetic model for chlorine decay. However, the document's primary focus is not on just modelling chlorine decay but on modelling DBP kinetics.

Chlorine decay is linked to DBP formation, prompting researchers to explore chlorine's role in DBP prediction. Furthermore, the influence of organic matter on chlorine decay is a critical factor. In this context, P. Hua et al., (2015) introduced a model that accounts for variable reaction rates to characterize chlorine decay in drinking water resulting from its interaction with dissolved organic matter. Ged et al., (2015), analysed the variability of 87 models from 23 different publications and highlighted that up until 2015, the main focus of most models had been on THM4 (Total Trihalomethanes).

However, there was a noticeable gap in the existing literature regarding models that evaluate total HAAs, specific THM and HAA species, bromate, and other DBPs that are not regulated. Selbes et al., (2018) explored the role of chloramine species in NDMA formation, Sathasivan et al., (2020) presented a dynamic model for THM species, Absalan et al., (2022) applied the variable reaction rate constant (VRRC) model to demonstrate its effectiveness in predicting chlorine decay and the formation of THMs in water containing ammonia during laboratory-scale experiments, while Premarathna et al., (2023) introduced a model for HAA formation. Abokifa et al., (2016a) developed a reactive-transport model involving multiple species to clarify the role of biofilms in the formation of DBPs. This model takes into account the concurrent transport and interactions of disinfectants, organic compounds, and biomass. To depict the interactions that occur between chlorine and TOC in aquatic systems, as well as the subsequent decay of chlorine and degradation of TOC, a basic model utilizing two components and second-order kinetics was employed by G. R. Abhijith & Ostfeld, (2022b). Further, they modelled THM formation from chlorine-TOC reactions by incorporating a reaction yield coefficient. G. R. Abhijith & Mohan, (2021) created a simple yet comprehensive model using EPANET-MSX to analyze the fluctuation of water quality over time and space in WDSs. The model takes into account the interplay

between chlorine, TOC, and bacteria, and is designed to be user-friendly and generic. Fisher et al., (2021) identified a fraction of fast-reacting substances as non-productive. They introduced models for TTHM formation, which include proportional models (representing the relationship between TTHM formation rate and chlorine demand by reactants) and productive models (indicating the contribution of fast and faster reactants to TTHM formation). These models encompass various chlorine reaction specifications, including single, two, and three-reactant models.

Zhao et al., (2018) investigated the variability of chemical reactions in drinking water distribution systems under different hydrodynamic conditions. The study employed three devices with varying wall demand and two types of NOM in the water to assess the changes in overall chlorine decay (k_O) and THM formation across stagnant to turbulent flow conditions. While many researchers have focused on modelling THMs, Yu & Reckhow, (2015) took a different approach and developed a model specifically for Haloacetonitriles (HANs). This model allows for quantitative predictions of HAN concentrations based on variations in pH and free chlorine contact times (CTs). In another study, X. Zhang et al., (2013) developed a kinetic model to simulate the formation of DBPs and investigate the effect of temperature. A regression model developed by Elshorbagy et al., (2000) for estimating THM level can be further considered as a dynamic model due to the incorporation of the time parameter.

Table 5: Chemical prediction models of DBPs in water distribution models

Disinfectant	DBP	Model	Reference
Chlorine	HAAs	$\frac{dC_{HAA9}}{dt} = Y_{HAA9} \times K_f \times C_f \times C_{Cl} + Y_{HAA9} \times K_s \times C_s \times C_{Cl}$	(Premarathna et al., 2023)
		$\frac{d(C_{HAA-Species})}{dt} = Y_{HAA-Species} \times (K_f \times C_f \times C_{Cl} + K_s \times C_s \times C_{Cl})$	
	THM	$C_{TTHM} = Y \times (C_{CL,0} - C_{Cl}) - Y \times C_{f,oth,0} + C_{TTHM,0}$	(Sathasivan et al., 2020)
	THM	$\frac{dC_{TTHM}}{dt} = Y \times K_{Cl} \times C_{Cl} \times \beta_b$	(Abokifa et al., 2016a)
	THM	$\frac{dC_{TTHM}}{dt} = M \times e^{N(\frac{-\Delta TTHM(t)}{\Delta TTHM_{max}})} \times Cl_2(t) \times (\Delta TTHM_{max} - \Delta TTHM(t))$	(Absalan et al., 2022)
	THM	$\frac{dC_{TTHM}}{dt} = Y \times K_{Cl} \times C_{TOC} \times C_{Cl}$	(G. R. Abhijith & Ostfeld, 2022a)
	THM	$\frac{\partial C_{TTHM}}{\partial t} + v\frac{\partial C_{TTHM}}{\partial x} = Y \times K_{Cl} \times C_{TOC} \times C_{Cl} + Y_\beta \times K_\beta \times \beta_h \times C_{Cl}$	(G. Abhijith et al., 2021)
	THM formation proportional	Single reactant: $\frac{dC_{TTHM}}{dt} = Y \times K_s \times C_s \times C_{Cl}$	(Fisher et al., 2021)
		Two reactant (2RA): $\frac{dC_{TTHM}}{dt} = Y \times [K_f \times C_f \times C_{Cl} + K_s \times C_s \times C_{Cl}]$	

Disinfectant	DBP	Model	Reference
	THM formation productive	Three reactant (3RA)-General: $\frac{dC_{TTHM}}{dt} = Y \times [K_f \times C_f \times C_{Cl} + K_{ff} \times C_{ff} \times C_{Cl} + K_s \times C_s \times C_{Cl}]$	
		Three reactant (3RA)-Simplified: $\frac{dC_{TTHM}}{dt} = Y \times [K_f \times p_{TTHM} \times C_f \times C_{Cl} + K_{ff} \times p_{TTHM} \times C_{ff} \times C_{Cl} + K_s \times C_s \times C_{Cl}] *$ $p_{TTHM} = \frac{(C_{f,0}+C_{ff})}{(C_{f,0}+C_{ff,0})}$**	
	THM	$C_{TTHM_{t+\Delta t}} = C_{TTHM_t} + 0.582(C_{Cl_{t+\Delta t}} - C_{Cl_t})$	(Elshorbagy et al., 2000)
	DBP	$C_{DBP} = C_{max}(e^{-k_d t} - e^{-k_p t})$	(X. Zhang et al., 2013)
	DBP	$C_{DBP} = C_{DBP,0} + \frac{k_{DBP} C_{E,0}}{k'_b + k_w} C_{Cl,0}(1 - e^{-k_o t})$	(Zhao et al., 2018)
Chloramines/ Chlorine	HAN	$\frac{dC_{HAN}}{dt} = -k_{H_2O} \times C_{HAN} - k_{OH} \times C_{OH^-} \times C_{HAN} - k_{HOCl} \times C_{HOCL} \times C_{HAN} - k_{ClO} \times C_{ClO^-} \times C_{HAN}$	(Yu & Reckhow, 2015)

C_{HAA9} is concentration of HAA, $C_{TTHM,0}$ is concentrations of total trihalomethanes before chlorine is dosed mg/L , C_{TTHM} Concentrations of total trihalomethanes at time t (h) in mg /L , C_{DBP} is temporal concentration profile of the DBP(mg/L), C_{max} is the maximum formation for each DBP during chlorination (mg/L), C_{TOC} concentration of TOC(mg/L), Y_{HAA9} is stoichiometric coefficient for HAA9 is assumed as α_{HAA9} for the reaction of chlorine with both FRA and SRA, $Y_{HAA-Species}$ can be expressed mgHAA-Species/mg-Cl_2. Can be changed by each other required HAA species. (Any other HAA species that is required can be substituted.) , Y is Yield of total trihalomethanes in [mg-TTHM/mg-Cl demand]/ reaction yield coefficient corresponding to THM formation from organic matter (mg/mg), Y_β reaction yield coefficient corresponding to THM formation from chlorination of biomass (mg-THM/mg-Cl), v flow velocity (m/s), x distance along the axial direction (m), K_f , K_{ff} and K_s are the reaction rate constants(decay rate coefficient) (L/mg Cl/h), K_{Cl} is the second-order reaction rate (L/mg organic carbon.s); β_b is the bulk biomass concentration (mg organic carbon/L), β_h Suspended biomass, K_β second-order kinetic constant corresponding to reactions between chlorine and biomass (L/CFU.s), k_d apparent reaction rate constants of DBP decomposition(1/h), k_p a new apparent production rate constant (which is the product of k'(reaction rate constants of DBP formation)and the stoichiometric ratio) (1/h), k_b' Kinetic constant for non-DBP forming chlorine decay, 1/hr, k_w Kinetic constant for the first order chlorine decay at wall, 1/hr, k_O Overall decay kinetic constant for chlorine, 1/hr, C_f and C_s are the concentrations (mg-Cl_2 equivalent/L) at time t (h) of FRAs and SRAs, respectively, C_{Cl} is the chlorine concentration (mg-Cl_2/L) at time t (h), $C_{f,oth,0}$ Initial concentration and fast-reacting agents that do not produce trihalomethanes in mg-Cl_2 /L, p_{TTHM} is the productive proportion of the fast and faster reactant ensemble(*,**) , M and N are model parameters describing the THMs formation rate, where M is expressed in (mg Cl_2/L)$^{-1}$h^{-1} and N is unitless,$\Delta TTHM(t)$ is the formed TTHMs at each time (µg/L), which equals $\Delta TTHM(t) - TTHM(0)$, $\Delta TTHM_{max}$ represents the maximum total THMs formation potential (mg/L), T time(h), C_{ff} are the concentrations (mg-Cl2 equivalent/L) at time t (h) of faster reactant, $C_{E,0}$ is the chlorine-molar equivalent of reactive NOM in water.

Table 6: Prediction absorbance and fluorescence models of DBPs in raw water

Type of water	DBP modelled (output)	Input parameters	Type of model	Scale	Reference
Raw water	DCAN and CPN	ΔUV_{272}, $\Delta(I_{500}/I_{450})$ and $\Delta\lambda^{em}0,5$	Differential absorbance model	Lab scale	(Roccaro et al., 2011)
Raw water	TCM, BDCM, MCAA, DCAA, TCAA, CH, DCAN and TCP	ΔUV_{272}	Differential absorbance model	Lab scale	(Korshin et al., 2002)
Raw water	THM4 and HAA9	ΔUV_{272}	Differential absorbance model	Lab scale	(Ates et al., 2007)
Raw water	THMs	ΔUV_{272}	Differential absorbance model	Lab scale	(Roccaro et al., 2008)
Raw water	TOX and THM	ΔUV_{272}	Differential absorbance model	Lab scale	(Korshin et al., 1997)
Raw water	TOX, TTHM, TCM, DCAA, and TCAA	ΔUV_{272}	Differential absorbance model	Lab scale	(C. W. Li et al., 1998)
Raw water and treated water	HANs	ΔUV_{272}, $\Delta(I_{500}/I_{450})$	Differential absorbance model	Lab scale	(Roccaro & Vagliasindi, 2010)
Raw and treated water	TTHM24h, and THAA24h	ΔFEEM	Differential absorbance model	Lab scale	(Roccaro et al., 2009)
Raw and treated water	THM, HAA, HAN	ΔFEEM	Differential ratio of fluorescence intensities or blue shift of normalized fluorescence spectra	Lab scale	(Roccaro et al., 2009)
Raw water and treated water	THMs, THAAs and DHAAs	ΔUV254-280	Differential absorbance model	Lab scale	(Yan et al., 2018)
Raw and treated water	TTHMs, HAAs	ΔFEEM	Differential ratio of fluorescence intensities	Lab scale	(Johnstone & Miller, 2009)
Raw and treated water	TTHMs,HAAs	ΔUV_{272}	Differential absorbance model	Full scale	(Beauchamp, Laflamme, et al., 2018)
Raw water, treated water and synthetic water	THM4, DCAA, TCAA and HAA6	ΔA (wide range of UVWavelengh)	Differential absorbance model	Lab scale	(Beauchamp et al., 2019)

4.2.2 Gaps and critical analysis

When building a model to solve complex problems, it's crucial to maintain simplicity instead of considering every factor and how they change. For example, a study investigating DBPs may choose to ignore temperature or chlorine variations and use just one set temperature and chlorine concentration for a more precise analysis as in Sathasivan et al., (2020). As a result, we need to re-examine our basic understanding to assess the rate at which each reaction occurs, including hydrolysis, the conversion of one DBP group (HAAs) to another (THMs), stability, and the transformation of one DBP species (e.g., $CHCl_3$) to another (e.g., $CHCl_2Br$). We also need to evaluate the yield formation of DBPs yet to be studied, under identical conditions.

In the various models introduced, certain shared assumptions are considered. These assumptions refer to parameters such as the chlorine concentration, the concentration of natural organic materials, and their kinetic rate constants. More specifically, these distinctions involve the classification of organic materials present in the water into two groups with different reaction rates, *fast* and *slow*, (Premarathna et al., 2023; Sathasivan et al., 2020), the presence of suspended or attached microbial film/mass (G. R. Abhijith & Mohan, 2021; G. R. Abhijith & Ostfeld, 2022b), the reaction rates, zero, first, or second order, (Gang et al., 2002; P. Hua et al., 2015; Premarathna et al., 2023; Sathasivan et al., 2020), the wall decay (Fisher et al., 2017; Premarathna et al., 2023; Sathasivan et al., 2020) and bulk decay coefficients (Fisher et al., 2017; Premarathna et al., 2023), the consideration of chlorine consumption by organic and inorganic compounds that do not result in DBP, namely, unproductive chlorine (Fisher et al., 2017; Premarathna et al., 2023), and environmental conditions, such as temperature (P. Hua et al., 2015; X. Zhang et al., 2013). The choice to incorporate or omit these assumptions in the models results in differences between them.

Upon careful consideration of the aforementioned points, it is apparent that numerous efforts have been made by researchers to enhance the accuracy and precision of these models. Despite these efforts, it's important to recognize that additional research is essential for a model to be applicable in a different water supply system or to enhance its overall applicability. New efforts should involve adapting the model to different water systems, types of DBPs, operating conditions, and seasonal variations. Carrying out these adjustments and refinements is crucial to make sure the model works well and can be trusted in a wide range of situations. Further, the application of absorbance and fluorescence models in WDN should be examined and the pros and cons between chlorine decay and spectroscopic based model should be further investigated.

5.0 MODELLING TOOLS IN WATER DISTRIBUTION NETWORKS

This section is dedicated to the comprehensive identification of existing water quality modelling tools, specifically focusing on multispecies reactive-transport (MSRT) models. These models intricately simulate the interactions and transport of diverse compounds, ultimately culminating in the formation of DBPs within WDSs.

As previously mentioned, key parameters such as water residence time and water demand traversing the distribution pipes profoundly influence DBP formation and overall water quality. Given their significance, proficient MSRT models must be conjoined with hydraulic analysis models. This integration produces a hydraulic state estimation for the analyzed system, a pivotal process that furnishes a comprehensive overview of the network. This encompasses water flows within each pipe, pressures at every node, consumer water demands, and tank levels (Vrachimis et al., 2018). Consequently, the conceptualization and creation of software tools capable of simulating the dynamic interplay of hydraulics and quality within WDSs have taken precedence (Clark, 2015).

5.1 Simulators

A noteworthy advancement in this direction was the introduction of EPANET software, an open-source hydraulic and quality simulator for water distribution systems, by the U.S. EPA (L. a Rossman, 2000). EPANET stands as the most widely utilized software for simulating hydraulic network operations, further supported by the "Open Water Analytics" community (https://github.com/OpenWaterAnalytics).

EPANET utilizes the "Gradient Algorithm" as proposed by Todini & Pilati, (1988) to replicate hydraulic dynamics. For quality modelling, it uses the Lagrangian time and event-based method introduced by Liou & Kroon, (1987) to solve hyperbolic partial differential equations. The quality simulator considers the mixing at junctions and tanks and the bulk and pipe wall reactions while it can model the advective transport and fate of just one chemical species with zero or linear dynamics (L. A. Rossman et al., 1993; L. a. Rossman & Boulos, 1996). To overcome these limitations, the EPANET-MSX software was developed as the multispecies expansion of the original EPANET, enabling the modelling of intricate interactions among multiple species while also accounting for dispersion processes (Shang et al., 2008).

Other known commercially available software used for DBP modelling are the WaterCAD and WaterGEMS tools developed by Bentley Systems (Bentley, 2023)

5.2 Integrating Risk Assessment, Early Warning and Simulation Tools

Due to their license status, the EPANET software and the EPANET-MSX extension have been integrated with various complementary toolkits. The EPANET-MATLAB toolkit, introduced by Eliades et al., (2016), offers the beneficial fusion of MATLAB's simulation capabilities with a variety of scenarios (G. Abhijith et al., 2021; Kyriakou et al., 2016). The EPANET-MSX engine has found application in multiple studies focused

on DBP formation. Kyriakou et al., (2016) developed the open-source dbpRisk toolkit, using EPANET-MSX dynamics to estimate THM formation risk by considering the quality dynamics between chlorine and TOC under different conditions and uncertainties, with a risk level being assigned to each node. In a more recent study, G. Abhijith et al., (2021) presented a comprehensive model encompassing bacterial regrowth and THM formation. This model examined 5 parameters including chlorine, TOC, biodegradable DOC (BDOC), bacteria, and THMs, factored in advective transport and intricate physicochemical and biological interactions. THM formation and bacterial regrowth were revealed by exploring the characteristics of source water and the residence time. Moreover, applications extended to designing booster chlorination stations to circumvent excessive THM production (Moeini et al., 2023; Ohar & Ostfeld, 2014), and evaluating nonlinear predictive control strategies considering chlorine-DBP interactions (Xie et al., 2018; Xie & Brdys, 2015).

Another notable advancement, EPANET-C, proposed by G. R. Abhijith & Ostfeld, (2022a), extends the EPANET-EPANET-MSX package for water quality simulation encompassing THMs. Integration of the EPANET-MSX modelling engine into software platforms not only aids decision-making and scenario exploration but also enhances monitoring interfaces. Such a system, which integrates sensor data and simulation models, is presented by Fattoruso et al., (2020) aiming to estimate the concentration of chlorine, THMS and HAAs. The proposed platform can be further used as an early warning mechanism since it consists of a GIS-based platform connected with field sensors measuring pressure, flow, and chlorine. Further, the system offers an optimal sensor placement strategy by utilizing a stochastic approach that considers a multi-objective optimization problem which takes into account the system's dynamic and known uncertainties.

Other simulation tools utilize 1-D models coupled with the EPANET (G. R. Abhijith & Mohan, 2021; Idornigie et al., 2010) or pilot-scale distribution system simulators (Abokifa et al., 2016a) for the formation and transport of DBPs within WDS. A multi-component reactive transport model, namely WU-MSRT was presented by Abokifa et al., (2016a) followed by a cellular automata-based mesoscale multispecies reactive-transport (CA-MSRT) developed by G. R. Abhijith & Mohan, (2021). Both models account for the advection and dispersion within water pipes to simulate the formation of THMs by considering the effect of biofilms and the interactions between chlorine, NOM and microbial biomass. The effect of temperature and various hydraulic conditions (e.g., flow) was further examined. The importance of considering dispersive transport is also highlighted since the models can simulate water quality in low-flow pipes and dead ends within the WDS. In Idornigie et al., (2010), the authors examined the impact of chlorine and water age in the formation of THMs and HAAs by coupling the EPANET simulator with two DBP formation models developed by Gang et al., (2002) and Sérodes et al., (2003).

Commercially, Bentley Systems' WaterCAD and WaterGEMS tools have been employed for DBP modelling (Bentley, 2023). In Chang et al.,(2010), the applicability of WaterCAD software was tested in predicting the THM and HAA concentrations while in Dias et al., (2017) a THM predictive model coupled with WaterGEMS for hydraulic

analysis was utilized to examine the transportation of THMs within District Metered Areas (DMA).

5.3 Water quality sensor placement

Apart from modelling and estimating the fate of DBPs in WDSs, models have been developed to enhance the monitoring capabilities of a system by defining strategies for optimal water quality sensor placement. The high cost of water quality sensors combined with the large-scale nature of WDSs makes the development of such monitoring strategies a necessary process for many water utilities. The water quality sensor placement strategy aims to identify the most suitable positions for installing the minimum number of online sensors with the objective of detecting a contamination event, estimating concentrations with the minimum error or detecting a change in water quality as quickly as possible. The quality dynamics of the target chemical species, the disinfection method, the network's topology and hydraulic assets and the water demands are necessary inputs for the development of an optimal sensor placement strategy.

Sensor placement is mainly considered an optimization problem evaluated using single or multi-objective approaches depending on the impact metrics. Such metrics can be the number of people affected, the detection time, the network coverage, the consumed contaminated volume, the detection likelihood, the risk of contamination etc. For the estimation of the optimal sensor placements, a variety of uncertainties (e.g., occurrence time, water flows, duration, type of chemical species) and probabilities (e.g., which section of the system is more likely to experience a water quality degradation) should be considered (Adedoja et al., 2018). The optimization solution can then be categorized into deterministic, stochastic and robust. A deterministic system can be described as a system where no uncertainties are taken into account when predicting the future state of the system. On the other hand, a stochastic system considers the existence of uncertainties, e.g., in water demands and the potential locations of a contamination. Monte Carlo samples are usually utilized to address these uncertainties, however, its accuracy depends on the assumptions made for the uncertainties distribution. Further, the effectiveness of the stochastic optimization approach is constrained by the need of having comprehensive and accurate distributional information regarding the contamination scenarios. In robust optimization, a worst-case cost is optimized within a defined uncertainty set without considering distributional information making this approach more realistic. A detailed review of existing sensor placement strategies can be found in Adedoja et al., (2018) and Eliades et al., (2023).

Generally, sensor placement strategies have been focused on identifying the best locations for sensors during the event of injected contamination (Q. Zhang et al., 2020) and considering more common water quality parameters such as chorine, pH, turbidity, dissolved oxygen and conductivity (Banna et al., 2014).

To the best of the author's knowledge, the investigation and application of sensor placement strategy focusing on DBPs monitoring and detection has not yet been addressed and generally remains unexplored.

5.4 Water Quality State Estimation

Dynamic state estimation, in this case, the water quality state estimation, is an important process that estimates the concentration of selected chemical species in space and time within WDSs. This process takes into consideration water quality dynamics, the hydraulic states derived from the hydraulic state estimation, and measurements from quality sensors. However, each of these sub-processes contains a level of uncertainty. Flow and velocity data can be inaccurate due to the unknown water demands used in the hydraulic state estimation process, quality dynamics focusing on estimating DBPs can be complex, and data from online sensors can include significant measurement noise. The issue of hydraulic uncertainties has been dealt with in several studies focusing on calibrating model parameters (Díaz et al., 2017) and minimizing the error from measurement and parametric uncertainties (Vrachimis et al., 2019; S. Wang et al., 2022).

Existing water quality state estimators mainly rely on chlorine measurements for validation with limited studies utilizing data from other types of sensors. Rajakumar et al., (2019), proposed a based-data assimilation technique using the ensemble Kalman filter (EnKF) to estimate chlorine concentrations while considering uncertainties regarding the source concentration and wall reaction coefficients. A different approach, presented by Vrachimis et al., (2021), calculates chlorine concentration bounds at nodes using hydraulic states, water quality model parameters, and real measurements as inputs to the proposed model. A quality state estimator considering DBPs has been introduced by Xie & Brdys, (2015), which utilizes the EPANET and EPANET MSX software for estimating quality states at space and time, however with the absence of real data for validation.

Concerning DBPs, more needs to be done. New methodologies should be developed concerning other disinfectants apart from chlorine, such as chlorine dioxide and chloramine, while utilizing new sensor data including UV and DOM measurements which are nowadays available.

6.0 STRATEGIES FOR OPTIMAL CONTROL

In this section, we focus on strategies aiming to control and reduce the DBP presence within WDNs. According to the literature, the main three points to control the DBPs are: water sources, water treatment plants, and water distribution. The following strategies and processes could be considered at each point:

In the water sources:

- Protection and monitoring of DOM/NOM levels

In water treatment plants:

- Disinfection control (type, dose and concentration) (Ao et al., 2020; Cheng et al., 2022; Godo-Pla, Rodríguez, et al., 2021; Maheshwari et al., 2020; Yuan et al., 2018; A. Zhang et al., 2019)
- Removal of DBPs precursors in raw water at the early treatment stage (Godo-Pla, Emiliano, et al., 2021; Z. Hua et al., 2019; Jutaporn et al., 2022; Park et al., 2019; Tak & Vellanki, 2018; Xing et al., 2019).
- Removal of DBPs in finished water at the late treatment stage (L. Wang et al., 2018; H. Yang et al., 2021)

In water distribution networks:

- Applying booster disinfection/operational interventions (Maheshwari *et al.*, 2018; Quintiliani *et al.*, 2017)
- Removal of DBPs as a point-of-use treatment (Chen et al., 2021)

Furthermore, there are some measures to reduce DBPs in drinking water based on the EPA advice such as improvements to raw water management, modification of the treatment process upstream of disinfection to improve the efficiency of THM precursor removal, optimization of the disinfection process, the use of alternative disinfectants for primary and secondary disinfection; and/or regular flushing and cleaning of storage reservoirs and distribution pipelines (The Environmental Protection Agency, 2013). It is necessary to mention that the effectiveness of these methods depends on the nature of precursors, the examined DBPs, water quality, operational conditions, financial issues, etc. In the following subsection we focus on control strategies that can be applied within WDN.

6.1 Literature review on optimal control of DBPs in WDN

A literature review was conducted focussing on identifying suitable strategies and technologies for DBP control and removal within WDN.

In Quintiliani et al., (2017), the authors suggested the manipulation of system actuators, such as opening/closing valves and hydrants and activating pumping stations for specific periods in order to minimize TTHMs concentrations in WDN. The proposed approach is considered a multi-objective optimization problem aiming to minimize the total number of operational interventions and the maximum TTHMs concentration observed at each network node over time. The problem is solved using the AMGA 2 optimizer[1], a C++ developed algorithm and the EPANET tool. However, depending on the case study, flushing of significant volumes of water is necessary which cannot be considered as a practical routine operational intervention.

In Maheshwari et al., (2018), a zone control approach combined with a decentralized optimization strategy, namely, the model coordination method, is suggested to combat the spatial complexity in WDNs and optimize the operation of booster chlorination. More specifically, the authors proposed the following methodologies:

[1] Archive-based Micro Genetic Algorithm

1. A data-based partitioning approach using principal components analysis (PCA) simplifies the spatial complexity of the network considering the disinfectant dosing rates at the nodes of the WDN.
2. A partial correlation analysis to assign disinfectant dosing rates to minimize interactions across subsystems.
3. The use of the effective relative gain array (ERGA) to verify minimal interactions.
4. A model coordination approach to facilitate coordinated decision making following the network partitioning.
5. An optimized-based formulation to maintain disinfectant residuals and water quality levels within the boundaries. This approach can take into consideration a network with more than one booster stations, which is partitioned based on the previous methodologies. For each subsystem which can be controlled by one or more booster their operation, the disinfectant dosage, can be optimized based on the following formulas:
    a. For the independent variable, U_j, (e.g., the subsystems' booster station disinfectant dosage rate):

$$\max_{U_j} \sum_{i=1}^{nd_j} (y_{ji} - y_l)^2 + (y_u - y_{ji})^2$$

and the constraints:

$$y_l \leq y_{ji} \leq y_u \;\; i = 1,2,3 \ldots nd_j$$

$$Y_{i,THM} \leq THM_{max}$$

$$y_l \leq U_j \leq y_u$$

where y_{ji} the chlorine residual concentration at each i^{th} node for each j^{th} subsystem, y_l the lower bound of chlorine residual concentration, y_u the upper bound of chlorine residual concentration, $Y_{i,THM}$ the calculated THM concentration, THM_{max} the maximum allowable THM concentration and U_j the disinfectant dosage concentration at j^{th} booster station.

    b. For the coordinating variables, U_x, (e.g., the disinfectant dosage rates from booster stations of other subsystems that affect the examined subsystem):

$$\max_{U_x} \sum_{i=1}^{nd_j} (y_i - y_l)^2 + (y_u - y_i)^2$$

and the constraints:

$$y_l \leq y_i \leq y_u \;\; i = 1,2,3 \ldots nd_j$$

$$Y_{i,THM} \leq THM_{max}$$

$$y_l \leq U_j \leq y_u$$

6. The use of an existing multispecies model for DBPs formation simulation.

In a more recent study by Maheshwari et al., (2020), an approach for optimizing the chlorination dosage while considering the limitation of microbial growth along with the simultaneous control of lead and DBPs in WDNs is presented. This challenge is considered as a multi-objective optimization problem aiming to achieve a balance between two competing goals: minimizing disinfectant dosage to reduce potential DBP formation while maximizing the supply of safe drinking water, considering both lead and residual free chlorine concentrations. A dynamic simulation-optimization framework that considers variations in network hydraulics and water chemistry, impacting lead and chlorine levels is utilized through a multi-objective genetic optimization algorithm integrated in a MATLAB-EPANET-MSX platform. The applicability of this approach is demonstrated in a real case study, where the optimal solutions, are visualized on Pareto plots. reveal the trade-offs between the 2 predefined objectives under different water chemistry conditions. These solutions include optimal disinfectant schedules for pumping and booster stations.

In a multivariate analysis, carried out by R. A. Li et al., (2022), the optimal re-dosing conditions of three key parameters of DBP formation, namely, the monochloramine dose (5 concentrations), pH (7 pH values) and bromide ion (3 concentrations) were investigated under variable water age. Using a series of multivariate bench-scale experiments. The optimization was carried out in a series of multivariate bench-scale experiments utilizing the Doehlert matrix. According to the results, to ensure monochloramine stability, it is recommended to employ a high monochloramine dosage (>1.5 mg-Cl2.L−1) in situations with moderate to high pH (pH = 7.8–8.0) and to minimize bromide concentration.

In a different study, Meyer et al., (2020) presented a method to compare the efficiency of different disinfection strategies, namely, booster chlorination, in-plant NOM removal, and distribution system granular activated carbon (GAC) adsorption and aeration. The authors used the relative health indication (RHI) that estimates the cumulative health risks regarding TTHM and HAA5 and produced population-weighted RHI values to quantify the impact of each strategy. The comparison was assessed by analysing the water-age dynamics of each strategy. According to the results, removing DBP precursors at the treatment plant is more beneficial for public health than the other methods applied within the distribution system. However, this difference between the impact of WTP and distribution strategies is attributed to the larger flows processed in WTP. When the population-weighted RHI is normalized for all strategies, it is demonstrated that disinfection strategies within distribution systems can have a significant impact. Better management of storage tanks and minimizing dead-end areas thus reducing water age are among the suggested improvements for these strategies.

J. Li et al., (2022), examined the effect of various factors regarding DBP formation and proposed several actions to mitigate their presence in WDNs. Regarding pipe material, the use of pipes with robust biological stability, such as polyethylene (PE) pipes, is recommended. Further, periodic biofilm removal, organic matter and bromide ion concentration reduction, control and removal of pipe wall biofilms and maintaining high flow rates can assist in DBP removal. In terms of disinfection methods, chlorine has proven more suitable for continuous disinfection compared to chloramine, although chlorine dioxide may emerge as a promising alternative in the future. Other disinfection methods include the use of PMS (peroxymonosulfate) as a disinfectant and the use of ultraviolet degradation technology (Q. Zhou et al., 2023). These methods, however, require more research to assess their long-term impact on water quality and public health.

In summary, ensuring high standards of water quality in WDNs is a complex task. It involves managing disinfectants, their degradation, corrosive by-products, interactions with biofilms, and methods for generating and removing DBPs. Balancing effective disinfection while minimizing harmful DBP formation remains an ongoing challenge, underscoring the importance of continued research in the field of drinking water safety.

7.0 CONCLUSIONS

In summary, this review underscores the need for more research focusing on DBP formation within WDN, improved replication of organic matter, a balanced focus on different DBP classes, the development of speciation models, and a shift toward mechanistic models. Applying these models to real-world water networks is crucial to ensure their effectiveness and reliability. Adapting models to various water systems, DBP types, operating conditions, and seasonal variations are essential for their applicability and trustworthiness across diverse scenarios. Addressing these gaps will contribute to a more comprehensive understanding of DBP formation and improve the safety of drinking water distribution systems.

Further, simplicity is essential for building dynamic models that simulate DBP formation due to the impracticality of considering all dynamic variables. Despite efforts to enhance accuracy, ongoing research is vital to extend a model's applicability across diverse conditions and water systems. Adaptations, involving different water systems, types of DBPs, operating conditions, and seasonal variations are crucial for reliable real-world use.

Sensor placement strategies have primarily concentrated on optimal locations for monitoring contamination events and common water quality parameters. However, the investigation and application of sensor placement strategies for DBPs remain unexplored. Further research is needed to address DBPs, including alternative disinfectants like chlorine dioxide and chloramine, and to leverage modern sensor data, such as UV and DOM measurements. This gap signifies the need for new methodologies in this critical area of water quality monitoring.

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intoDBP will create innovative tools and strategies to improve water quality management for safe human use and a healthy environment. It focuses on catchment protection and forecasting, transformative drinking water treatment, and real-time monitoring to combat the effects of climate and global change. In particular, intoDBP focuses on pollution and risks related to disinfection byproducts (DBPs). By developing and applying advanced, integrated, and cost-effective sensors and analytical methods, intoDBP will expand knowledge on water quality and DBP precursors to better understand its formation and human exposure in Europe. intoDBP monitoring results will feed into numerical forecasting tools to predict source water changes and formulate climate change adaptation pathways at catchment and treatment scale. intoDBP also develops transformative options for advanced and cost-effective upgrade of water treatment and disinfection.

In the intoDBP consortium researchers, small and large enterprises, communication experts and public services join forces to generate interdisciplinary solutions, that will generate a renewed perspective of drinking water surveillance, support decision-making and governance, and increase system resilience. intoDBP will implement and validate its cross-cutting products in four complementary case studies from three European countries where compliance with DBP regulation currently is an acknowledged challenge. The direct and visible positive impact of intoDBP in the case studies will foster rapid product adoption at a European and global scale, thus strengthening Europe's position and role in the global water market.

Reaching out beyond the water sector itself, intoDBP will directly engage society through surveys to analyze exposure to DBPs, collect data about catchment protection initiatives, create awareness and promote sustainable consumer behavior such as reducing bottled water consumption.

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