Formation of disinfection by-products (DBPs) in laboratory disinfection simulations under different experimental conditions

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Introduction

Among the biocidal active ingredients used for disinfection, highly reactive substances like chlorine, peroxides or ozone are common. During their application, numerous disinfection by-products (DBPs) are formed, especially if organic matter is present and may be released into the environment. This complex situation is not adequately considered in the guidance within the European Biocides Regulation at the moment. The existing "Guidance on Disinfection By-Products" [1] is limited to halogen-containing biocidal active substances (a.s.) and selected product types (PTs) and includes only general scientific strategies for the environmental risk assessment (ERA) of DBPs. The development of proposals to enhance the regulatory toolkit is the objective of the present project, sponsored by the German Environment Agency (UBA).

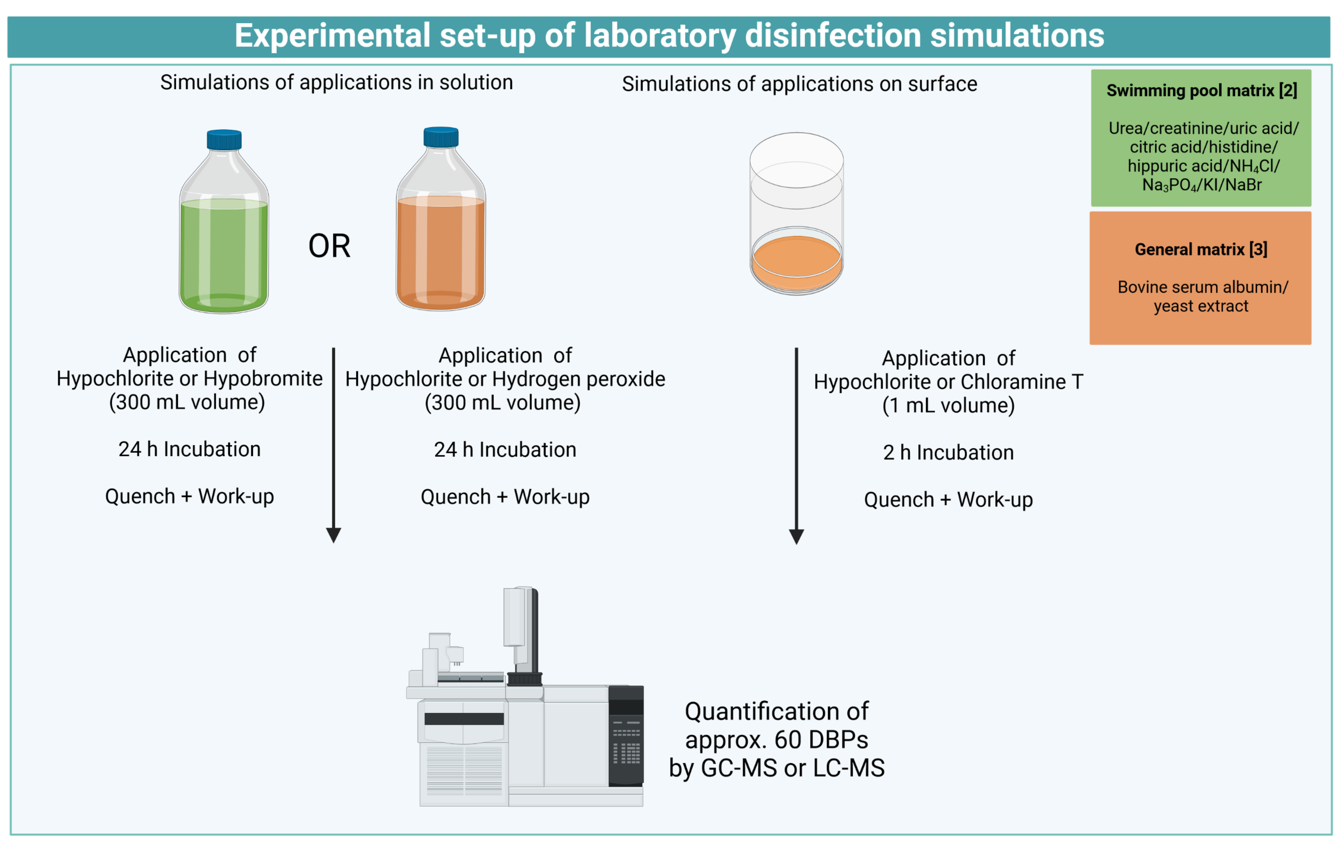
Main information gaps in literature

As a part the project, DBP related literature was searched for the time period 2013 - 2019. Two main information gaps were identified:

- DBP formation was found to be almost exclusively investigated for "chlorine-based" a.s. (chlorine, hypochlorite, chloramines accounted for approx. 90% of literature appearances)
- No information was available on DBP formation for surface applications, only disinfection uses in solution (mainly from PTs 2 and 5) are covered by literature

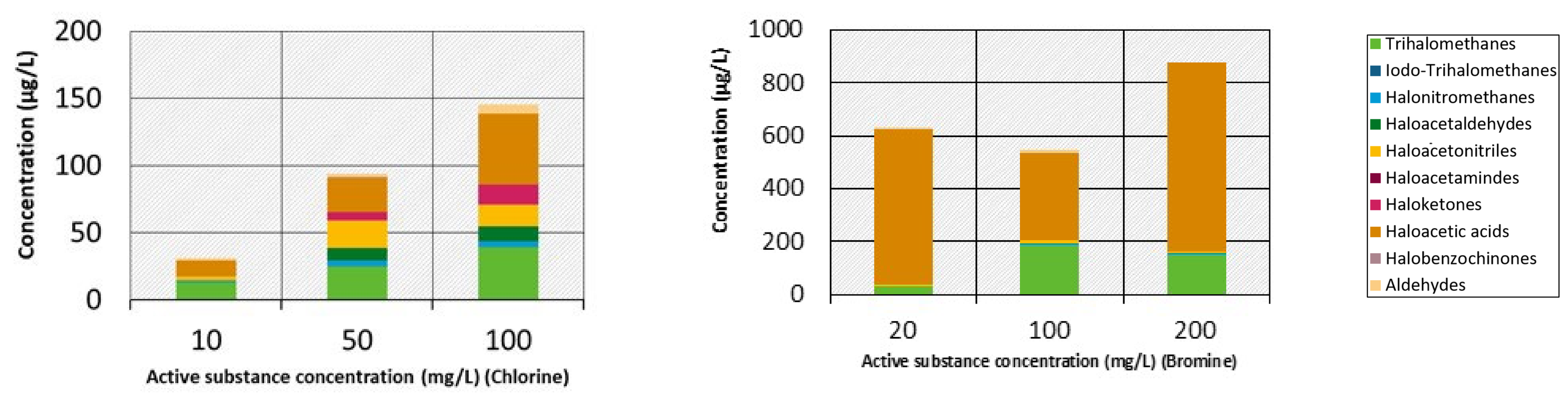
Materials and Methods

An important part of the project were laboratory simulations of disinfection applications including the analysis for a selection of approx. 60 DBPs. The disinfection simulations were performed using two matrix compositions, one focusing on disinfection uses in swimming pools and one containing organic matter that can be generally expected for uses across the regarded PTs 1-5, 11 and 12. Simulations were performed for uses in aqueous solutions and on hard surfaces. An elaborate dataset was generated by application of four different biocidal a.s. and the variation of different experimental parameters.



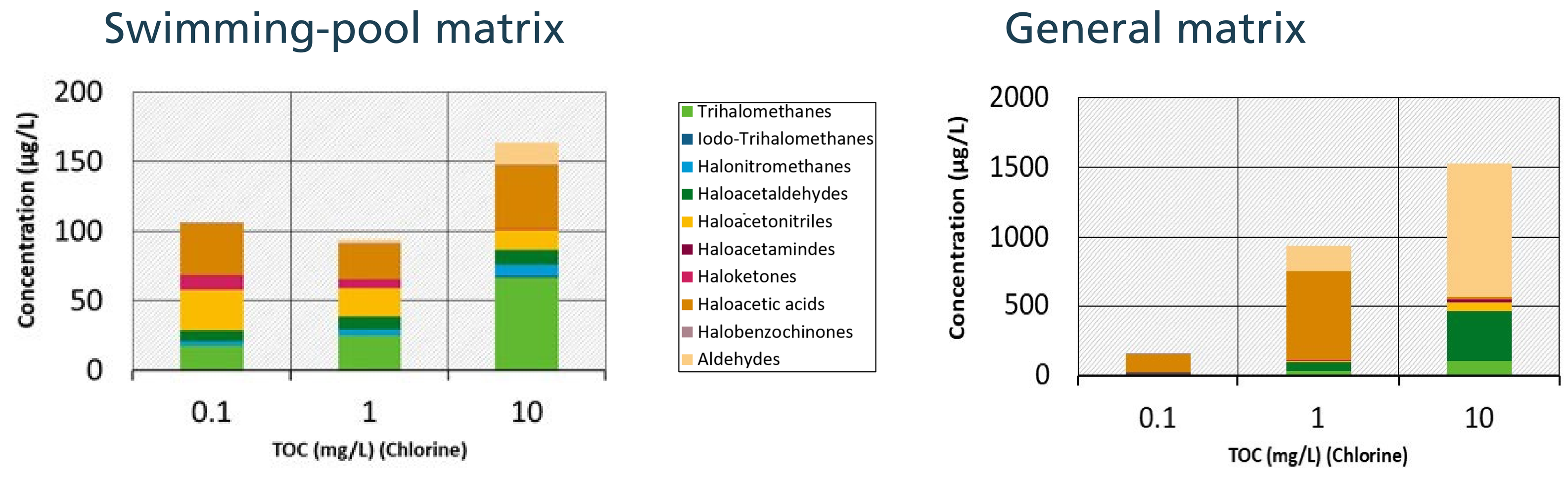
Results

Comparison of DBP classes after treatment of swimming pool matrix with hypochlorite or hypobromite

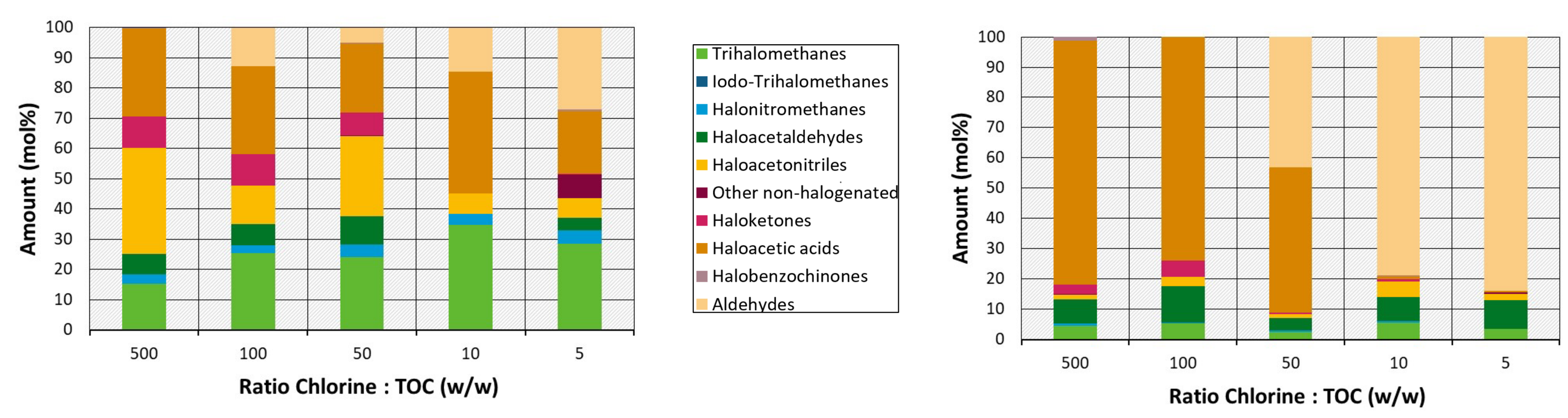


Treatment with HOCl results in large variety of different DPB classes. After treatment with HOBr only brominated THMs and HAAs are formed but at significantly high amounts.

Comparison of DBP classes after treatment of swimming pool or general matrix in solution with hypochlorite



Composition and amount of formed DBP differ significantly for the tested matrices, indicating that DBP formation will depend on the particular disinfection use. No systematic dependence for the composition of formed DBP for matrix concentrations is identifiable.



For general matrix (right) formation of some DBP families seem to depend on ratio chlorine:TOC (rather than the particular concentrations). HAAs are decreasing, aldehydes are increasing with decreasing chlorine:TOC ratio. Such correlation is not observed for the swimming pool matrix (left).

Differences after treatment of general matrix in solution or on surface with hypochlorite

Due to significantly differing reaction conditions, a direct comparison of disinfection simulations on surface and in solution is not reasonable. Additionally, results of surface disinfection simulations are limited because of losses of volatile DBPs.

Experimental condition	Simulation in solution	Simulation on surface
Chlorine amount (mg)	15	5
TOC amount (mg)	0.3	2
Incubation time (h)	24	2
Water volume (mL)	300	1

DBP	Simulation in solution	Simulation on surface
TCM, DCAA, TCAA, Trichloroacetaldehyde	High amounts	High amounts
Acetaldehyde	Major DBP	Minor DBP
Dalapon	Only traces	Major DBP
Monochloroacetic acid	Minor HAA	Main HAA

However, a qualitative comparison is possible and shows that the type of application leads to differences with respect to DBP formation. Some DBPs detected in disinfection simulations on surface and in solution are found at comparable rates but for others significant differences are observed.

Conclusion

Laboratory simulations show that DBP formation is a complex process involving not (completely) understood reaction chains differently influenced by reaction conditions. The performed target analytic of a limited DBP number could not explain all observations and deliver the "full picture". However, disinfection simulations show significant differences with respect to DBP formation when comparing the applied a.s. or the present matrix or the application type (solution or surface). To ensure a consistent and harmonised ERA of DBPs within the EU, first the identified information gaps need to be targeted. Subsequently detailed simulation designs, suitably covering all relevant uses, needs to be developed and included into the existing "Guidance on Disinfection By-Products" [1], if disinfection simulation data is intended to contribute to ERA of DBPs in the future.

[1] Guidance on the Biocidal Product Regulation, Volume V, Guidance on Disinfection By-Products, Version 1.0, January 2017.
[2] A. Kanan, T. Karanfil, Water Research, 2011.
[3] DIN EN 14885 (guidelines for efficacy studies on biocidal active substances).

Figure created with BioRender.

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