Investigation of disinfection byproduct formation during advanced water treatment using a transportable chemical reactor membrane inlet mass spectrometer

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When water is purified for drinking water by disinfection and/or polishing to eliminate pathogens and organic contaminants an unwanted formation of disinfection byproducts (DBPs) occurs. The type and amount of DBPs formed depends on both the water treatment technologies used and the specific chemical content of the water to be treated. To enable an on-site optimization of the water purification process, we are working on the development of an experimental laboratory reactor membrane inlet mass spectrometry system (ELR-MIMS) that can be brought to the waterworks for experimentation using site-specific raw water.

As a first step, we recently published [1] an algorithm for analyte quantification during water treatment in the ELR-MIMS using a combination of direct standard addition and an internal standard. Using this system, we were able to monitor and quantify the complex mixture of phenol, chlorinated intermediates and trihalomethanes produced during chlorination of phenols.

As a follow up, we have investigated the degradation of phenols by combined use of a biomimetic catalyst for advanced oxidation together with the chlorination. The catalyst, an iron(III) complex of the tetra-amido-N macrocyclic ligand (TAML) is oxidized by hypochlorite from its resting iron(III) stage into a reactive, high-valent iron(V) oxo species, which is capable of oxidizing persistent chemicals [2]. Our kinetic experiments demonstrated an extreme acceleration of the degradation of phenol, without any production of chlorinated intermediates and trihalomethanes using TAML concentrations higher than 1 µM (Fig. 1). Starting from low TAML concentration no effect was observed at concentrations < 0.005 µM, TAML concentrations between 0.005 µM and up to 0.1 µM caused increased reduction in chlorophenol intermediate concentrations but little effect upon trihalomethane production and at TAML concentrations above 0.1 µM a reduced trihalomethane concentration was also observed.
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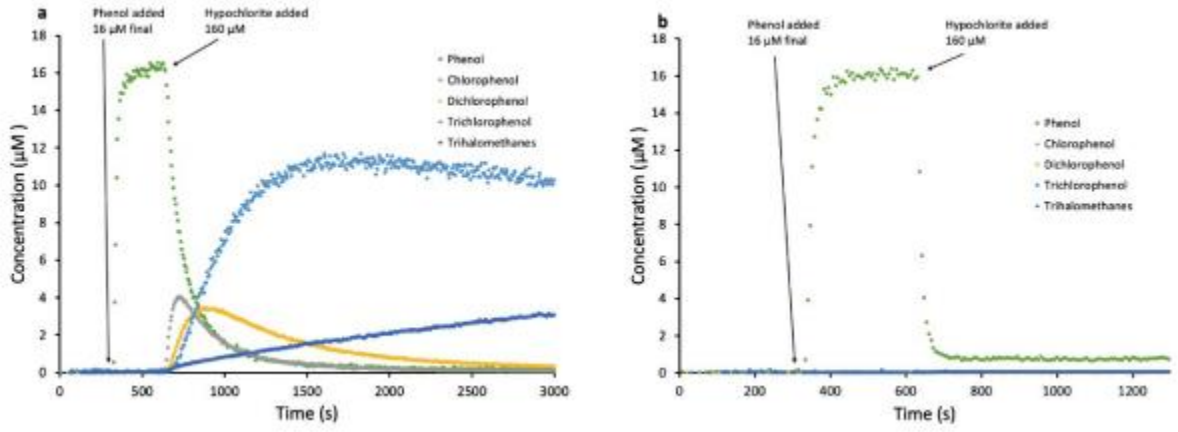

Figure 1. Monitoring of the degradation of phenol dissolved in (a) tap water using hypochlorite and (b) dissolved in tap water containing 66 µM of the catalyst TAML using hypochlorite.

References:

[1] F.T. Larsen, J.N. McPherson, C.J. McKenzie and F.R. Lauritsen. An experimental laboratory reactor for quantitative kinetic studies of disinfection byproduct formation using membrane inlet mass spectrometry. Rapid Communications in Mass Spectrometry 2022, 36, e9339.

[2] L.L Tang, M.A. Denardo, C.J. Schuler, M.R. Mills, C. Gayathri, R.R. Gil, R. Kanda, T.J. Collins. Homogeneous Catalysis Under Ultradilute Conditions: TAML/NaClO Oxidation of Persistent Metaldehyde. Journal of the American Chemical Society 2017, 139 (2), 879- 887.