Simultaneous MIMS and UV/VIS absorption for chemical reaction kinetic studies exemplified by disinfection byproduct formation from environmental contaminants

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Abstract

MIMS is a well-known method for online monitoring of volatile organic compounds and is highly suitable for online monitoring of volatile organic disinfection byproducts (DBPs) formed when water is disinfected, but it cannot analyze the typical precursor compounds (pesticides, pharmaceuticals etc.) to DBP formation. This problem can be overcome by simultaneous UV/VIS absorbance monitoring of the non-MIMS detectable precursor compounds simultaneous to MIMS monitoring of the formed volatile DBPs. In practice we use an experimental laboratory reactor (ELR) fully integrated with a membrane inlet mass spectrometer (MIMS) and a handheld UV/VIS spectrophotometer. This makes it possible to simulate the reactions that occur at waterworks when drinking water is disinfected.

As examples of reactions to simulate chlorination of contaminated water, we used some of the most common non-MIMS detectable water pollutants, acetaminophen (a pain reliever), caffeine (a lifestyle drug), and difenoconazole (a common herbicide). Acetaminophen is an example of a precursor that creates toxic short-lived intermediates (benzoquinones) that can be detected by both MIMS and UV absorption, caffeine is an example of a precursor that forms a wide range of highly toxic DBPs, and difenoconazole is an example of a precursor that barely responds to chlorination.

Some of the advantages achieved using the combined online MIMS – UV/VIS monitoring are:

- Knowledge about the quantitative fate of the non-MIMS detectable precursors to be used for understanding of mass balances.
- Independent UV/VIS verification of the identity of short-lived UV/VIS absorbing degradation intermediates.
- In connection with water chlorination, it often becomes possible to determine the amount of free chlorine, that is the amount of chlorine left for reaction with the DBP precursors after reaction with easy oxidizable constituents in the raw water investigated.

The benefits of simultaneous use of MIMS for monitoring of volatile organic compounds and UV/VIS absorbance for monitoring of non-MIMS but UV/VIS absorbing compounds can easily be transferred from laboratory studies using an ELR to field applications. This simply needs a MIMS with a flow-through membrane inlet where the aqueous sample passes through a small cylindrical cuvette before entering the thermostatically controlled membrane inlet.

Biography - Frants Lauritsen

Dr. Frants Roager Lauritsen, M.Sc., Ph.D., Dr. Scient. is professor at the Department of Physics, Chemistry and Pharmacy, University of Southern Denmark (SDU), and owner of the consultancy company MIMS Systems with expertise in design and implementation of mass spectrometers for on-site, on-line monitoring of chemical and biological processes. His recent work focuses upon disinfection byproduct formation in connection with water remediation.

Keywords

Combined MIMS and UV/VIS, Chemical reaction kinetics, Disinfection byproducts, Water contaminants