



Oxidation, aber richtig - preisgekrönte Dissertation

17. Juli 2024 | Andri Bryner

Themen: Trinkwasser | Abwasser | Schadstoffe | Institutionelles

Die Umweltchemikerin Joanna Houska ist für Ihre Doktorarbeit von der Deutschen Wasserchemischen Gesellschaft ausgezeichnet worden. Houska hat an der Eawag und EPFL geforscht und sowohl theoretisch als auch mit Experimenten aufgezeigt, wie die oxidative Behandlung von Wasser mit Ozon oder Chlor effizienter eingesetzt werden kann, wenn genauer bekannt ist, welche organischen Stoffe im zu behandelnden Wasser gelöst sind.

«Die Arbeit ist ein Meilenstein für ein besseres Verständnis der Rolle von gelöstem organischem Material bei der oxidativen Wasseraufbereitung», sagt Joanna Houskas Betreuer, Urs von Gunten. Er ist Professor an der EPFL und leitet am Wasserforschungsinstitut Eawag die Gruppe für Trinkwasserchemie. Houska verfüge, so von Gunten, über «eine enorme Fähigkeit, komplexe wissenschaftliche Fragestellungen theoretisch und experimentell zu bearbeiten und Probleme mit grosser Unabhängigkeit erfolgreich zu lösen.» In ihren Experimenten, aber auch mit Modellieren habe die Forscherin spannende neue Daten produziert und interpretiert, die zur Verbesserung der oxidativen Wasseraufbereitung eingesetzt werden können.

Ineffizient und gefährlich ohne genaue Analyse

Wo liegt denn das Problem? Werden Chlor oder Ozon zur Desinfektion/Oxidation von Wasser eingesetzt, ist das Hauptziel, Krankheitskeime und Mikroverunreinigungen unschädlich zu machen. Aber der grösste Teil der Oxidationsmittel reagiert mit Wassermatrixbestandteilen wie dem gelösten organischen Material. Das verringert nicht nur die Effizienz der Verfahren, sondern kann im dümmsten Fall zur Bildung von toxischen Nebenprodukten führen. Also sollte man möglichst genau wissen, was im zu behandelnden Wasser gelöst ist, um die Oxidation effizient zu machen. Hier hat Forscherin


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(15 chars) otherpage => protected'' (0 chars) categories => protected'dissolved organic
matter; oxidative titration; chlorine dioxide; ozone; elec
tron-donating capacity; molecular tagging; electron-rich moieties; phenols;
oxidation byproducts' (172 chars) description => protected'The application of oxidants for
disinfection or micropollutant abatement dur
ing drinking water and wastewater treatment is accompanied by oxidation of m
atrix components such as dissolved organic matter (DOM). To improve predicti
ons of the efficiency of oxidation processes and the formation of oxidation
products, methods to determine concentrations of oxidant-reactive phenolic,
olefinic or amine-type DOM moieties are critical.<br />Here, a novel selecti
ve oxidative titration approach is presented, which is based on reaction kin
etics of oxidation reactions towards certain DOM moieties. Phenolic moieties
were determined by oxidative titration with ClO<sub>2</sub> and O<sub>3</sub>

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b> for five DOM isolates and two secondary wastewater effluent samples. The determined concentrations of phenolic moieties correlated with the electron-donating capacity (EDC) and the formation of inorganic ClO₂-byproducts (HOCl, ClO₂[•], ClO₃[•]). ClO₂-byproduct yields from phenol and DOM isolates and changes due to the application of molecular tagging for phenols revealed a better understanding of oxidant-reactive structures within DOM. Overall, oxidative titrations with ClO₂ and O₃ provide a novel and promising tool to quantify oxidant-reactive moieties in complex mixtures such as

DOM and can be expanded to other matrices or oxidants.' (1422 chars) serialnumber => protected'0043-1354' (9 chars) doi => protected'10.1016/j.watres.2021.117790' (28 chars) uid => protected23921 (integer) _localizedUid => protected23921 (integer)modified _languageUid => protectedNULL _versionedUid => protected23921 (integer)modified pid => protected124 (integer) 1 => Snowflake\Publications\Domain\Model\Publicationprototypepersistent entity (uid=30070, pid=124) originalId => protected30070 (integer) authors => protected'Houska, J.; Manasfi, T.; Gebhardt, I.; von Gunten, U.' (73 chars) title => protected'Ozonation of lake water and wastewater: identification of carbonous and nitr

ogenous carbonyl-containing oxidation byproducts by non-target screening' (148 chars) journal => protected'Water Research' (14 chars) year => protected2023 (integer) volume => protected232 (integer) issue => protected'' (0 chars) startpage => protected'119484 (17 pp.)' (15 chars) otherpage => protected'' (0 chars) categories => protected'high resolution mass spectrometry; ozonation; carbonyl compounds; dissolved

organic matter; lake water; wastewater; phenols' (123 chars) description => protected'Ozonation of drinking water and wastewater is accompanied by the formation of disinfection byproducts (DBPs) such as low molecular weight aldehydes and ketones from the reactions of ozone with dissolved organic matter (DOM). By applying a recently developed non-target workflow, 178 carbonous and nitrogenous carbonyl compounds were detected during bench-scale ozonation of two lake waters and three secondary wastewater effluent samples and full-scale ozonation of secondary treated wastewater effluent. An overlapping subset of carbonyl compounds (20%) was detected in all water types. Moreover, wastewater effluents showed a significantly higher fraction of N-containing carbonyl compounds (30%) compared to lake water (17%). All carbonyl compounds can be classified in 5 main formation trends as a function of increasing specific ozone doses. Formation trends upon ozonation and comparison of results in presence and absence of the •OH radical scavenger DMSO in combination with kinetic and mechanistic information allowed to elucidate potential carbonyl structures. A link between the detected carbonyl compounds and their precursors was established by ozonating six model compounds (phenol, 4-ethylphenol, 4-methoxyphenol, sorbic acid, 3-buten-2-ol and acetylacetone). About one third of the detected carbonous carbonyl compounds detected in real waters was also detected by ozonating model compounds. Evaluation of the non-target analysis data revealed the identity of 15 carbonyl compounds, including hydroxylated aldehydes and ketones (e.g. hydroxyacetone, confidence level (CL) = 1), unsaturated dicarbonyls (e.g. acrolein, CL = 1; 2-butene-1,4-dial, CL = 1; 4-oxobut-2-enoic acid, CL = 2) and also a nitrogen-containing carbonyl compound (2-oxo-propanamide, CL = 1). Overall

compounds' (162 chars) journal => protected'Water Research' (14 chars) year => protected2023 (integer) volume => protected237 (integer) issue => protected" (0 chars) startpage => protected'119751 (14 pp.)' (15 chars) otherpage => protected" (0 chars) categories => protected'carbonyl compounds; disinfection byproducts; ozonation; dissolved organic ma

ter; non-target analysis; high-resolution mass spectrometry' (136 chars) description => protected'Ozonation of natural waters is typically associated with the formation of carbonyl compounds (aldehydes, ketones and ketoacids), a main class of organic disinfection byproducts (DBPs). However, the detection of carbonyl compounds in water and wastewater is challenged by multiple difficulties inherent to their physicochemical properties. A non-target screening method involving the derivatisation of carbonyl compounds with p-toluenesulfonylhydrazine (TSH) followed by their analysis using liquid chromatography coupled to electrospray ionisation high-resolution mass spectrometry (LC-ESI-HRMS) and an advanced non-target screening and data processing workflow was developed. The workflow was applied to investigate the formation of carbonyl compounds during ozonation of different water types including lake water, aqueous solutions containing Suwannee River Fulvic acid (SRFA), and wastewater. A higher sensitivity for most target carbonyl compounds was achieved compared to previous derivatisation methods. Moreover, the method allowed the identification of known and unknown carbonyl compounds. 8 out of 17 target carbonyl compounds were consistently detected above limits of quantification (LOQs) in most ozonated samples. Generally, the concentrations of the 8 detected target compounds decreased in the order: formaldehyde > acetaldehyde > glyoxylic acid > pyruvic acid > glutaraldehyde > 2,3-butanedione > glyoxal > 1-acetyl-1-cyclohexene. The DOC concentration-normalised formation of carbonyl compounds during ozonation was higher in wastewater and SRFA-containing water than in lake water. The specific ozone doses and the type of the dissolved organic matter (DOM) played a predominant role for the extent of formation of carbonyl compounds. Five formation trends were distinguished for different carbonyl compounds. Some compounds were produced continuously upon ozonation even at high ozone doses, while others reached a maximum concentration at a certain...' (2551 chars) serialnumber => protected'0043-1354' (9 chars)

doi => protected'10.1016/j.watres.2023.119751' (28 chars) uid => protected30345 (integer) _localizedUid => protected30345 (integer)modified _languageUid => protectedNULL _versionedUid => protected30345 (integer)modified pid => protected124 (integer) Houska, J.; Salhi, E.; Walpen, N.; von Gunten, U. (2021) Oxidant-reactive carbonous moieties in dissolved organic matter: selective quantification by oxidative titration using chlorine dioxide and ozone, *Water Research*, 207, 117790 (11 pp.), [doi:10.1016/j.watres.2021.117790](https://doi.org/10.1016/j.watres.2021.117790), [Institutional Repository](#)

Houska, J.; Manasfi, T.; Gebhardt, I.; von Gunten, U. (2023) Ozonation of lake water and wastewater: identification of carbonous and nitrogenous carbonyl-containing oxidation byproducts by non-target screening, *Water Research*, 232, 119484 (17 pp.), [doi:10.1016/j.watres.2022.119484](https://doi.org/10.1016/j.watres.2022.119484), [Institutional Repository](#)

Houska, J.; Stocco, L.; Hofstetter, T. B.; Gunten, U. von (2023) Hydrogen peroxide formation during ozonation of olefins and phenol: mechanistic insights from oxygen isotope signatures, *Environmental Science and Technology*, 57, 18950-18959, [doi:10.1021/acs.est.3c00788](https://doi.org/10.1021/acs.est.3c00788), [Institutional Repository](#)

Manasfi, T.; Houska, J.; Gebhardt, I.; von Gunten, U. (2023) Formation of carbonyl compounds during ozonation of lake water and wastewater: development of a non-target screening method and quantification of target compounds, *Water Research*, 237, 119751 (14 pp.), doi:10.1016/j.watres.2023.119751, [Institutional Repository](#)

Links

Promotionspreis

Eawag Forschungsgruppe Trinkwasserchemie

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