

UNIVERSITÄT
DUISBURG
ESSEN



2019

Jahresbericht
Annual Report

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Instrumental Analytical Chemistry



Dear friends and colleagues,

2019 has been a year in transition in many regards that will become truly effective in 2020. Sadly, we have to mourn the loss of two colleagues in our faculty, our long-term dean Carsten Schmuck and our dear external colleague in analytical chemistry Hans-Georg Schmarr who both died this summer. The former also led to my election as dean of the faculty of chemistry in October that kept me quite busy since. Furthermore, I have been newly elected as review board member for analytical chemistry at the German Science Foundation (DFG). And after almost a year of proposal discussion we hope that UDE in January 2020 will officially announce a fifth research profile area in water research that I am designated speaker of. The proposal for the DFG Collaborative Research Centre RESIST (led by Bernd Sures) has passed the first step of the evaluation and next year in September we will have the final on-site evaluation in Essen. Another big change will happen at IWW Water Centre, where the long-term CTO Wolf Merkel will leave for a new position at DVGW. With the current research coordinator at IWW, David Schwesig, we have surely found a good replacement. At the end of 2019 I would specifically like to say thanks to my fabulous team at IAC that helps to master all the mentioned changes and new challenges. One of the long-term team members, Dr. Holger Lutze, will leave us though in 2020 to take over a professorship at the TU Darmstadt. Congratulations for that promotion, Holger! We wish you all the best for your future! After many years of successful work at IAC we hope that we can continue with a close collaboration but of course this causes further changes within IAC, and a milestone next year will be the appointment of a new group leader in our group.

Of course, we also worked hard throughout the year. As a result, we have published almost as many papers in international journals than last year (27), many of which appeared in the premier journals of the field. Several new projects were granted and commenced in 2019 that will be summarized in an overview of running projects on the next pages to give you an idea of our current activities at the university. Not included here but very important as part of the group activities are the projects by external PhD students at IWW, IUTA and various other research institutes and in industry.

Four PhD students finished successfully their theses and were awarded their doctoral degrees. 7 Master and 6 Bachelor students finished their thesis at our department or at an external partner institutes with a home supervisor at IAC. In addition to the annual meeting of the Water Chemistry Society in Erfurt in May, we have been heavily involved in the organization of the 8th Late summer workshop of the Water Chemistry Society in September. Finally, I would like to thank again all group members and students for their excellent work at IAC and all partners from academia, industry and funding agencies for their great support and fruitful collaborations.

I hope you are interested in our IAC report and wish all of you the best for 2020. We welcome very much feedback or collaboration interests for the future.



Torsten C. Schmidt



Instrumental Analytical Chemistry Group Members (autumn 2019)

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Head of Chair

Prof. Dr. Torsten C. Schmidt

Secretarial Office

Lydia Vaaßen

Regular Staff

Dipl.- Ing. Gerd Fischer	Project Administration, IT Administrator
Dr. Maik Jochmann (AOR)	Stable Isotope Analysis/Sample Preparation and Gas Chromatography
Dr. Klaus Kerpen	2D-Fluorescence Spectroscopy/Advanced Oxidation Processes/Laser Commissioner
Dipl.- Ing. Robert Knierim	Laboratory equipment/Glassware/Support of guest scientists
Dr. Holger Lutze	Advanced Oxidation Processes
Robert Marks	Technical support
PD Dr. Ursula Telgheder	Ion Mobility Spectrometry/2D-Fluorescence Spectroscopy/Expert advice for course of studies/Radiation Protection Commissioner
Claudia Ullrich	Laboratory assistant/Safety officer

Apprentices

Anna Spehr	Laboratory assistant
Tessa Luise de Kock	Laboratory assistant

Ph.D. Students

Internal

Mohammad Sajjad Abdighahroudi	An investigation of Pharmaceutical and Personal Care Products (PPCPs) as potential precursors for Nitrogenous Disinfection Byproduct (N-DBPs)
Christian Becker	Response analysis for a newly developed flame ionization detector for liquid chromatography
Tobias Hesse	Liquid chromatographic methods for stable isotope analysis
Lotta Hohrenk	Suspect and non-target screening of diffuse immissions into aquatic systems
Katharina Hupperich	Influence of organic matter on oxidative transformation processes
Sasho Joksimoski	Novel coupling techniques for the determination of organic compounds in complex samples by ion mobility spectrometry
Wiebke Kaziur-Cegla	Development of a generic protocol for automated sample preparation in GC-MS
Daniel Köster	Development of a wet-chemical interface for online nitrogen isotope analysis of organic compounds using liquid chromatography-isotope ratio mass spectrometry (LC-IRMS)
Nerea Lorenzo Parodi	Aromatic amines as biomarkers in human urine: Analytical method development and epidemiological studies
Seyed Mohammad Seyed Khademi	Development of an on-line monitoring system for the analysis of organic contaminants in aquifers based on ion mobility spectrometry
Valentina Merkus	Characterization of transformation processes using high-resolution mass spectrometry
Xenia Mutke	Treatment of membrane concentrates by oxidative processes
Manuel Stephan	Microextraction techniques in GC/IRMS
Nenad Stojanovic	Development and application of advanced stable isotope methods to study compound degradation at real field sites
Jens Terhalle	Transformation processes and Isotope effects in natural and technical aqueous systems
Laura Wiegand	Characterisation of reactive species in the Fenton reaction
Sarah Willach	Stable isotope analysis to characterize oxidative and photochemical transformation processes

Vanessa Wirzberger	Oxidative water treatment: mechanistic aspects and matrix effects
Cornelia Zscheppank	Development of an analytical method for Identification and fast Screening Analysis of Microbial Metabolites

External

Anastasia Barion (Günter)	Disk SPE-based sensitive determination of organochlorine pesticides and polybrominated diphenyl ethers in water
Nico Bätz	Effect-directed identification and reduction of diffuse immissions in rivers
Sandro Castronovo	Examination of micropollutant degradation in biological wastewater treatment: a proteomics approach
Matthias Dumm	Cyanides in furnace gas scrubbing slurry
Matin Funck	Development of a Sampling-Procedure allowing subsequent qualitative and quantitative Pyrolysis-GC/MS analysis for Sub μ -Plastics in the Aquatic Environment
Lina Gessner	Evaluation of a simple quantification method of drugs of abuse in dried blood spots
Vanessa Hinnenkamp	Development and application of suspect and non-target screening of water samples using high resolution mass spectrometry (HRMS)
Oliver Höcker	Characterisation of anaerobic processes in biogas generation using non-target screening
Fabian Itzel	Evaluation of innovative wastewater treatment processes using instrumental and effect-based analysis
Sarah Klaes	Development and optimization of an electrochemical flow cell and coupling with the multi-elemental analysis
Kjell Kochale	Automated hyphenation of effect-based and instrumental analysis
Susann Pristat	Development of procedure tests for hot and cold coils considering the optimization of transport logistics of slabs
Kirsten Purschke	Suspected Target Screening of organic compounds in industrial wastewater
Lars Reinders	Monoclonal Antibodies in Occupational Hygiene Surveillance
Gerrit Renner	Development of new spectroscopic and multivariate chemometric methods for the characterisation of (micro)plastics in the marine environment

Sara Schäfer (Saß)	Oxidative transformation of organic compounds in ultrapure water by ozonation and UV photolysis
Tobias Uber	Adsorption and desorption processes on polymers in aquatic systems
Tobias Werres	Microfluidic characterisation of high performance liquid chromatography systems with the main emphasis on the intrinsic efficiency

Research and Teaching Assistants

Katharina Hupperich

Mischa Jütte

Hyerin Kim

Valentina Merkus

Simon Nikutta

Christina Sommer

Felix Niemann

Guest Scientists



Prof. Sina Dobaradaran, Bushehr University of Medical Sciences, Iran

- Comprehensive study on environmental emissions/sorption of PAHs by cigarette butts (CBs)
- Study of the kinetics of PAHs release from the cigarette butts into the aqueous solutions
- Improvement of a method for detection of PAHs contents of CBs by GC-MS (my next project)



Prof. Hiroto Kawashima, Akita Prefectural University, Japan

Areas of Specialty:

- Stable Isotope Analysis
- Environmental Science/Forensics
- Pesticide, VOCs, aerosol



Dr. Cheolyong Kim, Pusan National University, South Korea

Formation mechanisms of halogenated by-products from dissolved organic matter (DOM) during the sulfate radical based oxidation process



Prof. Maryam Vosough, Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran

In this academic visit and in continuation of the previous collaboration, performance of multivariate chemometric methods such as multiway, unsupervised and supervised classification methods for high throughput nontarget screening (NTS) of organic micropollutants in river and wastewater treatment plant effluent samples using full scan LC-HRMS/MS measurements, was investigated. In this regard, the role of chemometric tools to process MS/MS data at two acquisition strategies of data-dependent and data-independent analysis was also studied. Another important aspect of NTS in environmental samples is prioritization of unknown compounds, which was implemented in this study and another similar work by utilizing different extraction strategies and significant time-trend fluctuations, respectively.



Prof. Amir Salemi, Shahid Beheshti University, Tehran, Iran

The main goal of this academic visit, and the second collaboration with Prof. Torsten C. Schmidt and his scientific staff, was to further examine the analytical capabilities of direct immersion PAL SPME Arrow technique, following summer 2018 joint research. Phosphorus flame retardants, an important class of emerging contaminants, were target analytes and the extraction parameters were optimized using a central composite response surface methodology. Satisfactory results were achieved regarding analytical figures of merit, such as sensitivity, linearity, precision and accuracy. A river sample (Ruhr, Essen) was also investigated to examine capability of the method in more complex matrices and some of the target analytes were detected in the sample. It was showed that PAL SPME Arrow was significantly superior over other published methods, especially for its sensitivity, low sample volume requirement, robustness and solvent free nature.

Awards



Nerea Lorenzo-Parodi

Nomination for the Agnes and István Halasz Young Scientist Award 2019 at ANAKON (March 25, 2019) for her lecture “Aromatic amines in human urine: automation and optimization of the sample preparation”



Dr. Holger Lutze

Award of the Water Chemistry Society, Erfurt, May 27, 2019 for his outstanding work on a mechanistic understanding of oxidative processes in water treatment.



Dr. Oliver Knoop

Young Scientist Award 2019, Centre for Water and Environmental Research (ZWU) for his PhD thesis „Formation and Effects of Transformation Products during the Ozonation of Tamoxifen“
(Essen, May 21, 2019)



Xenia Mutke

Young Scientist Award 2019, Centre for Water and Environmental Research (ZWU) for her master thesis „Investigation of reactions of saturated heterocyclic amines with chloride“
(Essen, May 21, 2019)



Xenia Mutke

Water Science Awards for best master theses:
„Investigation of reactions of saturated heterocyclic amines with chloride dioxide”
1st Venator Water Award)
Essen, December 09, 2019

Xenia Mutke investigated the reactions of the heterocyclic amines piperazine and piperidine with chlorine dioxide. The complex study included the determination of second-order reaction constants of these compounds with hypochlorous acid and chlorine dioxide, the reaction stoichiometry and the formation of chlorine by-products. Furthermore, she investigated the reaction of cetirizine with chlorine dioxide, as an example of structural related pharmaceutical with a piperazine moiety.



Valentina Merkus

Best master degree in Water Science
Essen, November 13, 2019



Valentina Merkus

Water Science Awards for best master theses:

„Analysis of transformation products during the ozonation of nitrogen containing compounds in presence of matrix constituents with LC-HRMS“

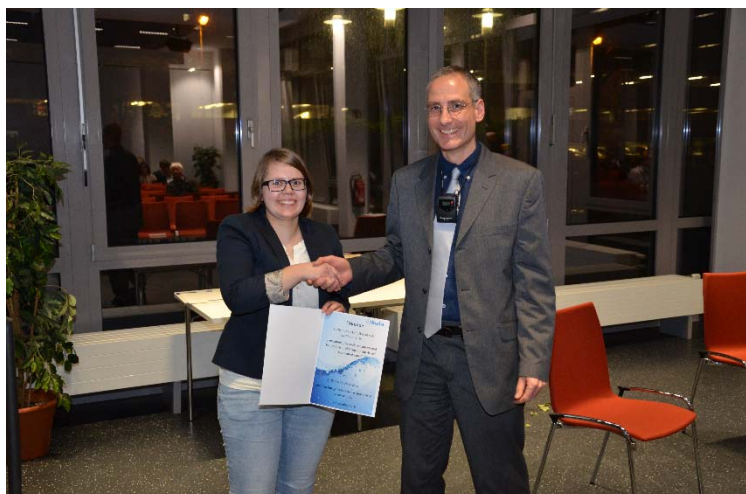
2nd Venator Water Award
Essen, December 09, 2019

Ozonation is one applied method in waste water treatment for removal of micropollutants. During this reaction transformation products are formed, which cause harmful effects in the environment. The formation of these products is highly dependent on the water matrix. Valentina Merkus investigated the influence of matrix constituents on transformation products of two nitrogen containing example compounds.



Valentina Merkus

On December 09, 2019 Valentina Merkus was awarded for best performance in analytical chemistry during the Water Science Master program by Mikheil Gogiashvili (GDCh, Division of Analytical Chemistry).



Katharina Hupperich

Water Science Awards for best master theses:

„Formation of secondary oxidants and by-products in chlorine dioxide-based treatment of water” (Kurita Award)

Essen, December 09, 2019

Katharina Hupperich investigated the inorganic by-product formation in chlorine dioxide treatment of natural organic

matter (NOM). Thereby, she studied model compounds as surrogates for functional groups in NOM as well as Suwannee River NOM and determined the yields of chlorite, chloride, chlorate and hypochlorous acid, which can act as a secondary oxidant.



Dr. Sina Dobaradaran

Award for the best poster at the 3rd International and 21nd National Conference on Environmental Health
Zanjan, IRAN. February 02, 2019

Running Projects at IAC 2019

NRW Graduate School Future Water: Global water research in the metropolitan region Ruhr (Future water)

Involved staff: Lotta Hohrenk (IAC PhD student), Vanessa Wirzberger (IAC PhD student), Dr. Holger V. Lutze, Claudia Freimuth (Coordinator), Prof. Dr. Torsten C. Schmidt (Speaker)

Involved students: Valentina Merkus, Michelle Klein

Partners: Prof. Dr. Bernd Sures, Prof. Dr.-Ing. André Niemann, Prof. Dr. Martin Denecke, Prof. Dr. Rainer Meckenstock, Prof. Dr. Jens Boenigk, Prof. Dr. Nicolai Dose (University of Duisburg-Essen), Prof. Dr. Marc Wichern (Ruhr-University Bochum), Dr. Jochen Türk, Fabian Itzel, Nico Bätz (IUTA), Prof. Dr. Sigrid Schäfer, Dr. Daniel Dangel (EBZ Business School Bochum), Prof. Dr. Mark Oelmann (HRW Mülheim), Dr. Steven Engler (KWI Essen) and many mentors and collaborators from the water and wastewater sector

Funding: Ministry for Culture and Science of the State of North-Rhine Westphalia (NRW) through the joint project “Future Water: Global water research in the metropolitan region Ruhr”



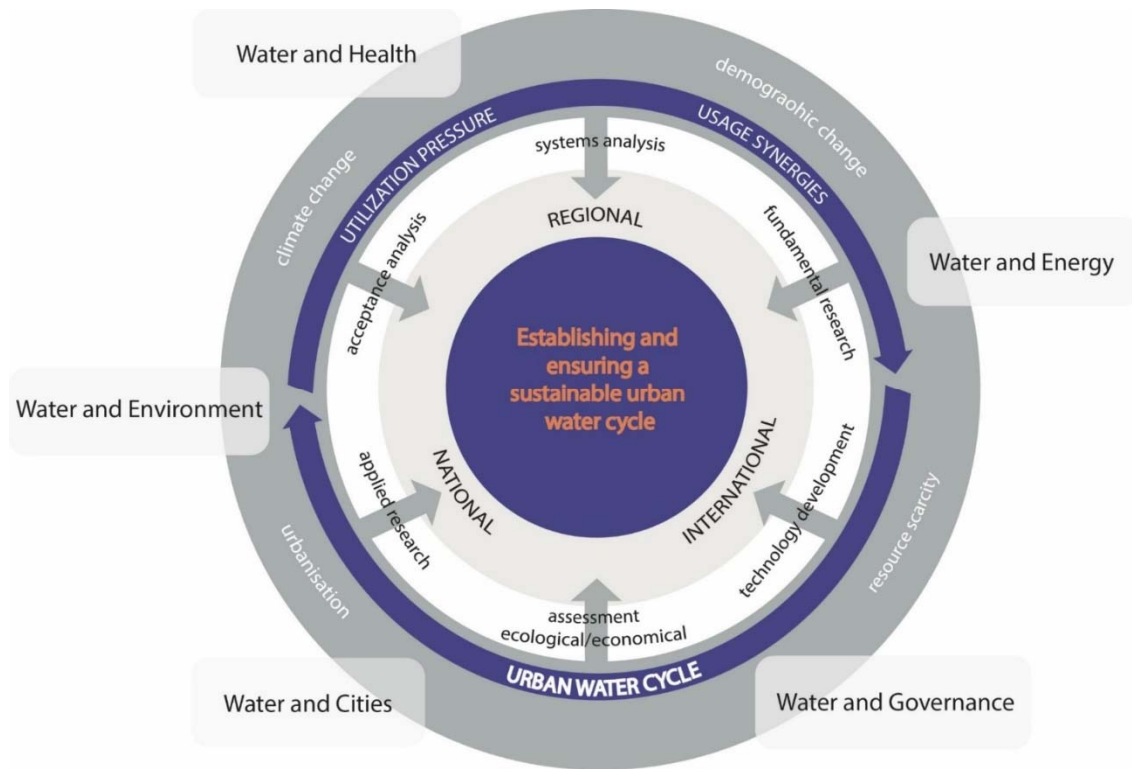
The multiperspectivity of inter- and transdisciplinary approaches allows to conduct innovative and path-breaking research. Combining knowledge and methods across disciplines makes possible to identify hitherto unnoted research questions. Tackling questions from different and novel angles allows to find answers that have not been conceived before. The integration of practitioners into these processes can enhance the relevance of the research questions, the fit of the methods applied, the effectiveness of research processes and the applicability and outreach of the results.

This approach is at the very heart of the graduate school “Future Water”, which is located in the Ruhr metropolitan area in Western Germany.

In 2014, a variety of academic and applied institutes joined forces to develop strategies for a sustainable water management with a special focus on the urban water cycle. The following figure describes the many facets of that work. The wide array of disciplinary backgrounds represented in the graduate school made building bridges between the natural sciences, applied engineering and social sciences both possible and necessary. Altogether, in Future Water 12 PhD students and a coordinator position are funded. Coordination is done by the Centre for Water and Environmental Research (ZWU) at UDE.

At IAC, one project focuses on the analysis of micropollutants introduced by diffuse sources with nontarget screening. Nontarget screening is based on high resolution mass spectrometry and offers the potential of detecting broad range of analytes at low concentration in one full scan measurement. By that it provides a more comprehensive overview about compounds present in a sample, enables the identification of formerly unknown contaminants and reveal temporal or spatial trends.

Another project at IAC that is associated to the future water graduate school deals with reaction mechanisms of nitrogen containing compounds (in detail diclofenac, metoprolol and isoproturon) during ozonation with special focus on the reaction with matrix components and the formation of transformation products. Transformation products are identified with LC-HRMS and tested in regards of their toxicity to aquatic organism (*D. magna*).



Advanced chemometrics to optimize LC-HRMS approaches for suspect and non-target screening of emerging pollutants in water samples

Involved staff: Lotta Hohrenk, Prof. Dr. Torsten C. Schmidt

Partners: Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran

Funding: German Research Foundation (DFG)

DFG funded a seed project to initiate international collaboration with the group of Prof. Maryam Vosough, Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran (see also under guest scientists). Maryam visited Essen in summer 2018 and 2019 for two months each.

Main results were:

Considering production of the massive data during LC-HRMS measurements of the environmental samples and the necessity to extract as much information as possible from the data, implementation of chemometric tools are highly necessary. Different chemometric mining methods can be employed or developed for different steps of a screening workflow such as proper background correction, peak detection, peak resolution, time-shift correction and feature prioritization before an identification step.

In the current collaborative study, multivariate deconvolution and supervised classification of highly complex and mixed signals obtained through LC-HRMS measurements was performed as a start point. The deconvolution method of choice was multivariate curve resolution-alternating least squares (MCR/ALS). The pronounced advantage of this algorithm is that one can retrieve the pure profiles of components even in the presence of retention time shifts and shape changes of components between different chromatographic runs. So, a chromatographic peak alignment step is not necessary anymore. Also, in contrast to most data processing strategies, which focus on analyzing each m/z channel at a time and extracting ion chromatograms and grouping the features belonging to the same compound, multiway methods are able to simultaneously decompose the entire data matrices into the pure chromatograms, pure mass spectra and the relative quantities of all systematically oriented signals in different sample data matrices. This can be very useful for reducing feature redundancy. This resolution process was considered for both targeted and nontargeted parts of the mentioned collaborative study.

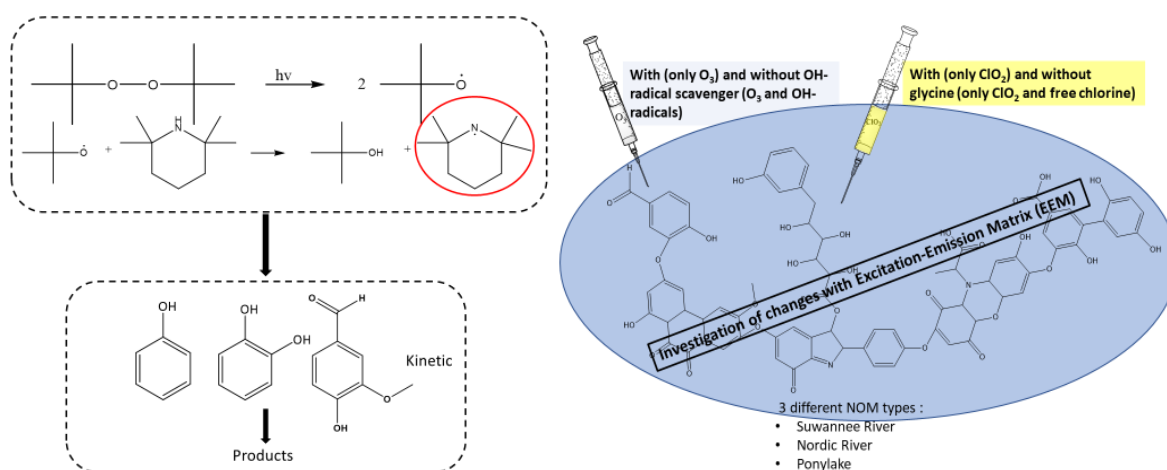
Influence of organic matter on oxidative transformation processes

Involved staff: Katharina Hupperich, Dr. Holger V. Lütze

Funding: German Research Foundation (DFG)

It was shown that matrix components can affect the transformation product formation during oxidative processes. This was firstly observed in the transformation of dimethylsulfonamide to the cancerogenous compound *N*-nitrosodimethylamine (NDMA) which required the presence of bromide. Currently, such effects of the water matrix on transformation processes are hardly investigated. The present project deals with matrix effects on transformation processes governed by natural organic matter (NOM). In oxidative water treatment NOM is the main consumer of the oxidant and these reactions can form reactive species which could contribute in pollutant transformation. One of these reactive intermediates are aminyl and nitroxyl radicals, which are barely studied yet and therefore, this is one major task in the present project.

Thereby, kinetics of the reaction with aminyl radicals with simple model compounds representing reactive sites of pollutants will be investigated. Furthermore, structural changes in different NOM types upon reactions with oxidants will be investigated using excitation emission measurements (EEM).



Left: Formation of aminyl radicals and their reaction with model compounds, right: experimental concept of EEM measurements.

Membrane processes in drinking water supply (KonTriSol)

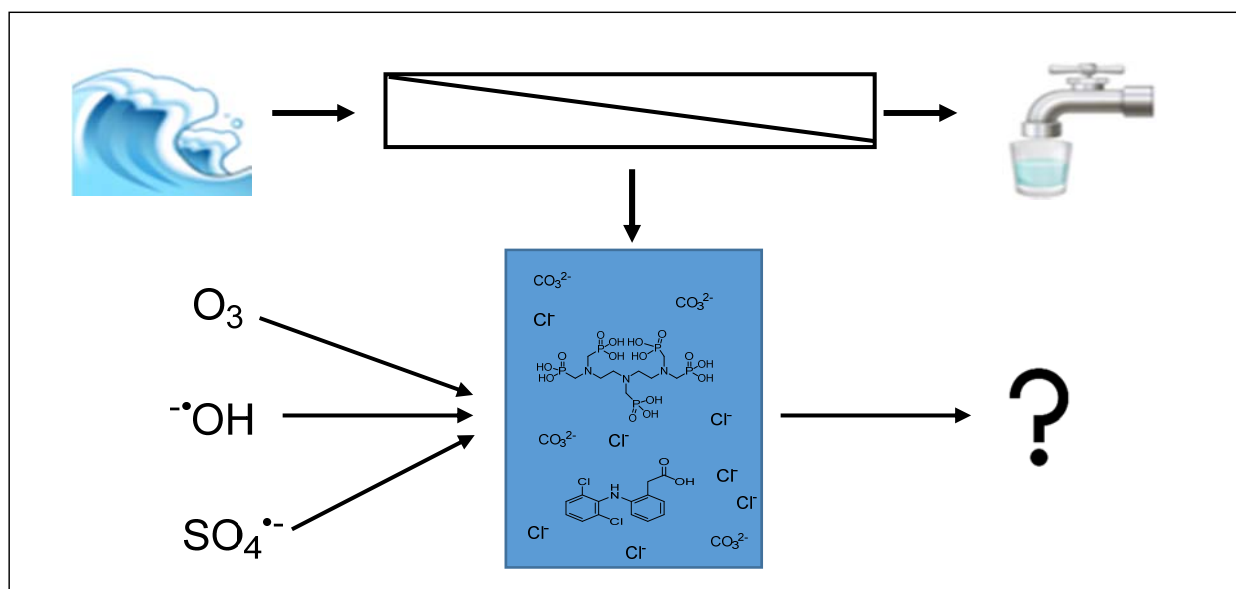
Part: Membrane concentrate treatment with oxidative processes

Involved staff: Xenia, Mutke, Dr. Holger V. Lutze, Prof. Dr. Torsten C. Schmidt

Partners: IWW Water Centre, TZW, University Frankfurt, Technical University Berlin, Technical University Hamburg-Harburg, Cornelsen Umwelttechnologie, Delta Umwelt-Technik, Lagotec, Lanxess, Solenis,

Funding: Federal Ministry of Education and Research (BMBF)

The project KonTriSol deals with the technical, legal and economic solution approaches for the usage of nanofiltration (NF) and reverse osmosis (RO) processes. Over the next years, ten project partners will work on elimination steps for technical and permission barriers of NF/RO technology in drinking water treatment.



NF and RO membrane technologies enabling the reduction of water hardness, inorganic water constituents, natural organic substances and anthropogenic substances. The resulting concentrates contain a high concentration of these substances and additionally a high concentration of antiscalant chemicals added during the treatment processes. The direct disposal of concentrates to the environment could be hazardous to aquatic organisms and increase the micropollutant contamination of water bodies.

The aim of the IAC project part is to investigate the application of oxidative processes to concentrates of membrane processes. Focus of the study is the reactivity of antiscalants in regard to different oxidizing agents like ozone, hydroxyl radicals and sulfate radicals. Furthermore, the influence of high matrices (high chloride, nitrate, carbonate content) on the degradation efficiency of antiscalants, pharmaceuticals and perfluorinated compounds will be investigated.

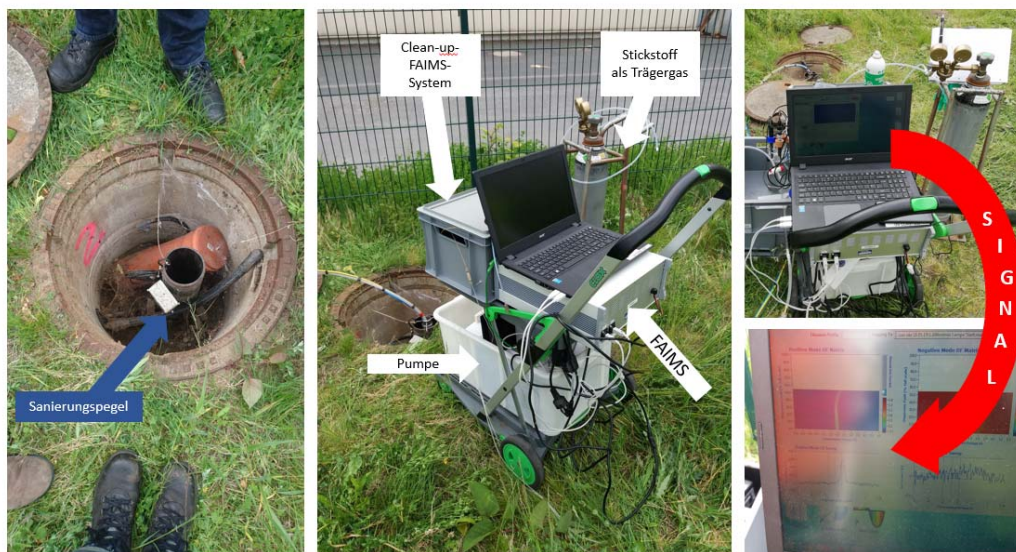
Development of a combined in-situ-remediation- and monitoring system for the treatment of groundwater damages (LUKE)

Involved staff: Sasho Joskimoski, Michelle Lüling, PD Dr. Ursula Telgheder

Involved students: Dionysios Tzimis

Partners: Fabricius Pro Terra GmbH

Funding: Federal Ministry for Economic Affairs and Energy (BMWi) by the Central Innovation Programme for SMEs (ZIM)



Installation of the analysis system at Arsol Aromatics, Gelsenkirchen

In-situ remediation and monitoring of groundwater damage will increasingly replace the classic pump and treat systems in the coming years, since these can often no longer work economically due to the reduced amount of pollutants. In addition, there are increased environmental requirements and advanced analytics, with which even low loads can still be detected and may fall under the obligation to remediate. At the same time, better analytical monitoring of the damage events is sought in order to document the success of the remediation. A combination system consisting of a floor lance, gas injection and on-site analysis would enable efficient renovation at reduced costs and simple installation. These initial considerations led to the basic idea of this project.

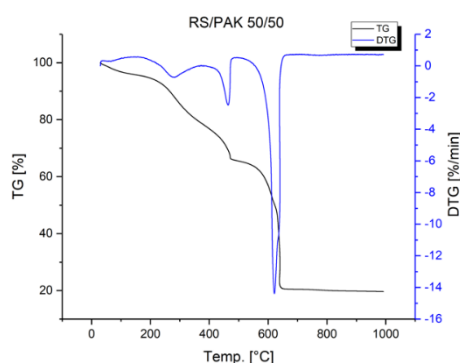
A special multi-parameter lance system was developed for the introduction of the gas injection system, for sampling and for the direct determination of the parameters pH, O₂ content, conductivity and moisture in the aquifer. The renovation is carried out by the reversible introduction of a glass fiber reinforced polymer membrane into the aquifer, which releases oxygen in a diffusive way. A modified FAIMS spectrometer is coupled with the system, which allows continuous monitoring of the pollutant concentration at the observation level. After optimizing the experimental parameters, the multi-parameter lance system was tested in field trials. The modified FAIMS spectrometer was validated by regular sampling from selected levels and subsequent GC-MS analysis in the laboratory.

“Den Spurenstoffen auf der Spur – Teil 3” (DSADS)

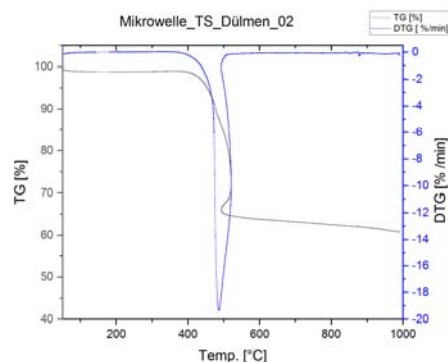
Involved staff: PD Dr. Ursula Telgheder

Partners: Lippe Verband, Ruhr-Universität Bochum, Fachgebiet Siedlungswasser- und Abfallwirtschaft Universität Duisburg – Essen, Fakultät für Biologie, Abteilung Aquatische Ökologie Universität Duisburg - Essen

Funding: District Government Münster, North-Rhine Westphalia



Differential mass loss thermograms of thermal decomposition of dry substances (Return sludge (RS) / Activated carbon powder (PAK))



Differential mass loss thermograms of thermal decomposition of dried return sludge from the contact basin in Dülmen after pyrolysis

The aim of this project is the development of a reliable method for evaluation of the suitability of the application of activated carbon as a 4th purification step in waste water treatment. Up to now, it is not known if a small proportion of the loaded activated carbon is passing the sand filter or is released into the water bodies.

When sampling water containing PAHs, sampling using scooping samples is recommended, since the activated carbon can adhere to plastic hoses. This would falsify the sample.

Thermogravimetry has proven to be a suitable method for determining PAHs in water. The majority of the organic accompanying substances can be located between $T = 170\text{ °C}$ and 430 °C and the PAK signal at approx. 600 °C .

A sensitivity increase can be achieved by combining microwave ashing with thermogravimetry. The organic components are pyrolyzed in the microwave before analyzed by thermogravimetry.

The figure above shows the result of a thermogravimetry analyses of a pyrolyzed sample from the contact basin in Dülmen. No significant maximum mass losses are observed in the lower temperature range between $T = 170\text{ °C}$ and 430 °C , which would correspond to organic accompanying substances. Furthermore, the baseline is significantly reduced (by approx. 10%) and the PAK signal can be recognized at approx. 530 °C without interference by interfering signals. These results lead to the conclusion that, firstly, a significant proportion of PAH is contained in the samples from the contact basin (sampling point 3) (20% / min) and secondly, the combination of microwave ashing - thermogravimetry leads to a separation of the interfering substances. Thus, the sensitivity of the procedure is improved.

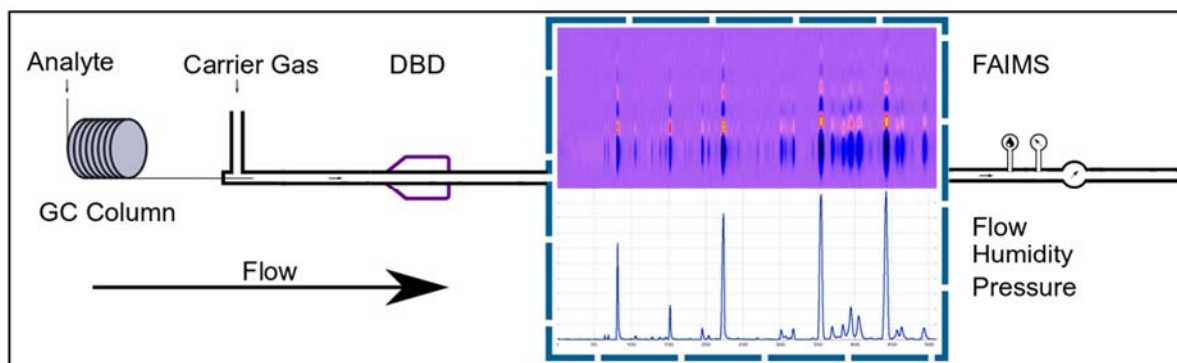
Multi-Ion - Non-radioactive, energetically variable ionization unit for fast and selective pollutant analysis in building materials based on FAIMS technology

Involved staff: Dr. Klaus Kerpen, Fabian Ude, Robert Marks, PD Dr. Ursula Telgheder

Involved students: Marina Braum

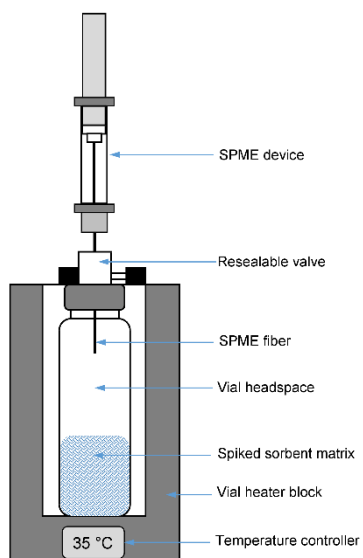
Partners: Schumann Analytics GmbH

Funding: Federal Ministry for Economic Affairs and Energy (BMWi) by the Central Innovation Programme for SMEs (ZIM)



Schematic set-up of GC-DBD-FAIMS system

The aim of this project is to develop a non-radioactive, energetically variable ionization unit which (Dielectric barrier discharge (DBD), in combination with Gas Chromatography (GC) - Ion Mobility Spectrometry (FAIMS), enables the rapid on-site analysis of toxicologically relevant substances in both older, previously used (waste wood) as well as in new construction products (mostly modern insulation materials). Important steps to characterize the non-radioactive source were the creation of simple and stable gas standards over a longer period of time. The selected analytes were added to a standard sample vessel filled with silicone oil (polyhenylmethylsiloxane and polydimethylsiloxane) and heated at a constant temperature until equilibrium is reached. Then the gas space above the suspension is sampled with a micro-extraction fiber for a definite time. An exact temperature control of these filled sample vessels should ensure a constant concentration of the respective substances in the gas phase at all times. These constant concentrations are fed to the overall system by means of micro-extraction and subsequent thermal desorption and are currently used to check the optimization steps on both non-radioactive ionization units and the overall system.



Calibration system

Development of an LC-IRMS interface for the component specific determination of the nitrogen isotopic ratios of organic compounds via wet chemical oxidation/reduction (LC-IRMS)

Involved staff: Daniel Köster, Tobias Hesse, Dr. Maik A. Jochmann, Dr. Holger V. Lutze, Prof. Dr. Torsten C. Schmidt

Funding: German Research Foundation (DFG)

Compound-specific isotope analysis (CSIA) of carbon by LC-IRMS is a widely applied method to investigate food authenticity or to get insights into transformation and degradation processes. The system is designed to oxidize compounds to CO₂ by wet chemical oxidation using persulfate, which limits its current application to carbon isotope measurements. The goal of this project is to make the system also suitable for CSIA of nitrogen, which requires several modifications and new methods to evaluate oxidation efficiencies during conversion and extraction.

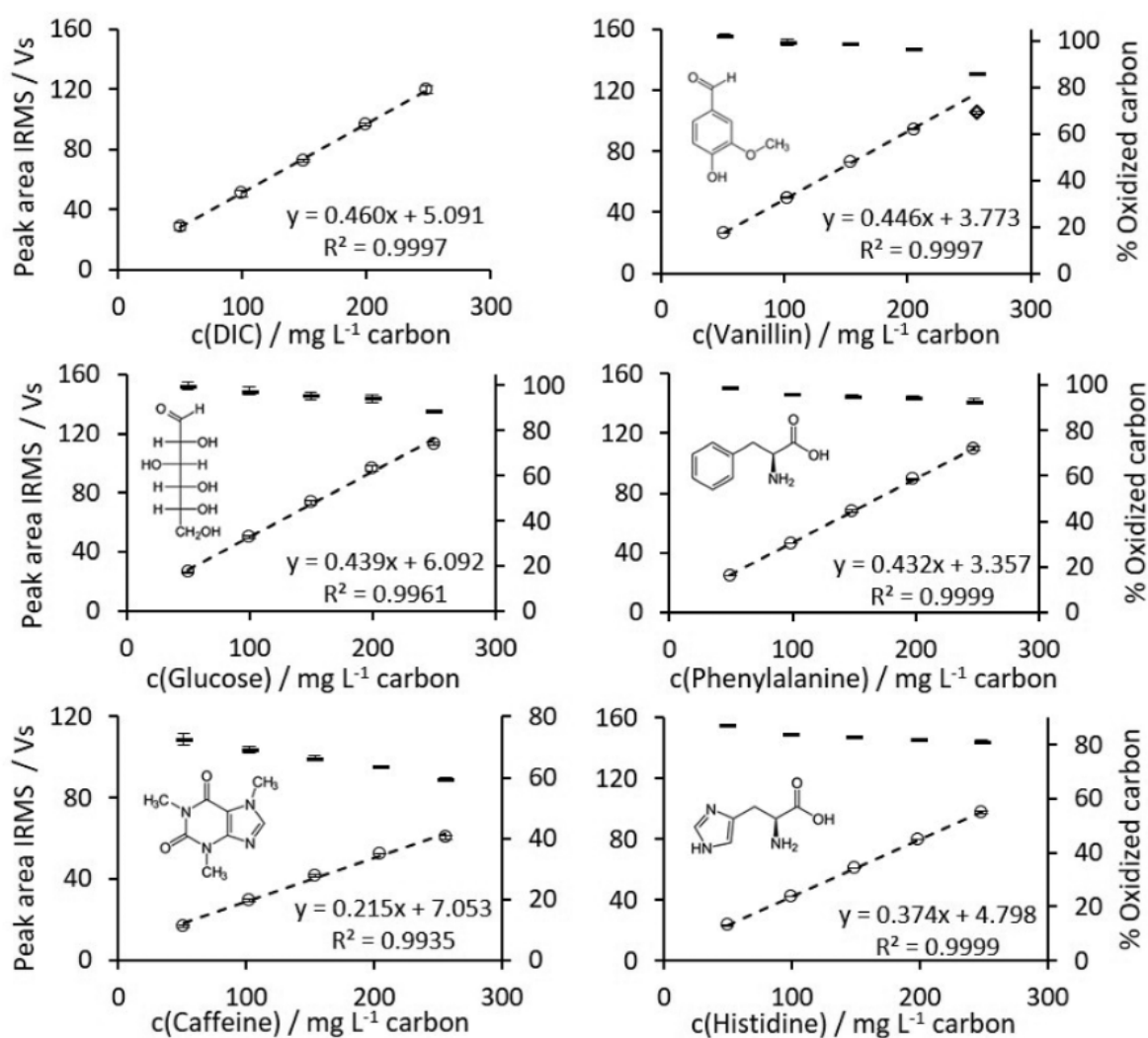


Figure 1: Peak area obtained by IRMS analysis and oxidation efficiencies plotted against carbon concentration of common LC-IRMS analytes (flow injection). Circles indicate peak areas on the first y-axis, horizontal bars indicate oxidation efficiencies on the second y-axis.

It was shown that regular concepts to evaluate oxidation efficiencies e.g. by linear area response curves are not suitable to accurately assess oxidation rates (Figure 1). While the linear regression of the response area plotted against carbon concentration indicate no direct change in the oxidation

efficiency on its own ($R^2 > 0.99$), comparing the slopes of the linear regression to inorganic carbon standards (DIC) showed differences especially for compounds containing N-heteroatomic systems such as caffeine and histidine. The slope of DIC standards over a range of 50 to 250 mg L⁻¹ of carbon was 0.460 Vs L mg⁻¹, whereas identical carbon concentrations for caffeine and histidine had a lower slope of 0.215 Vs L mg⁻¹ and 0.374 Vs L mg⁻¹. Comparing the peak areas of DIC to the individual compounds of the same concentration furthermore showed incomplete oxidation rates even for compounds such as glucose or vanillin, which are easier to oxidize.

Further changes were related to the investigation of the fundamental oxidation and mineralization mechanism of nitrogen containing compounds. Not much was known about the mineralization end products formed during wet chemical oxidation by sulfate-radicals. For an in-depth investigation and complete characterization of the mineralization products, methods had to be developed that were able to determine a nearly complete nitrogen mass balance. In this context, methods based on TOC/TN_b as well as TOC/IC were combined and evaluated. Fundamental investigations of the acidic wet-chemical oxidation processes with sulfate-radicals showed that compounds without aromatically bound nitrogen will be oxidized to ammonium as main product in a fast reaction. A further oxidation to nitrate was not observed. Special difficulties appeared during the oxidation of compounds containing N-heteroaromatic systems. These compounds were far more difficult to oxidize and the main mineralization products were ammonium and nitrate in the same proportion. Additionally, it turned out that the mass balance was not complete (Figure 2). The acidic wet chemical oxidation by persulfate is therefore not applicable for LC-IRMS of nitrogen. However, oxidation under alkaline conditions showed mineralization yields of higher than 95% for all nitrogen containing compounds with nitrate as the only product.

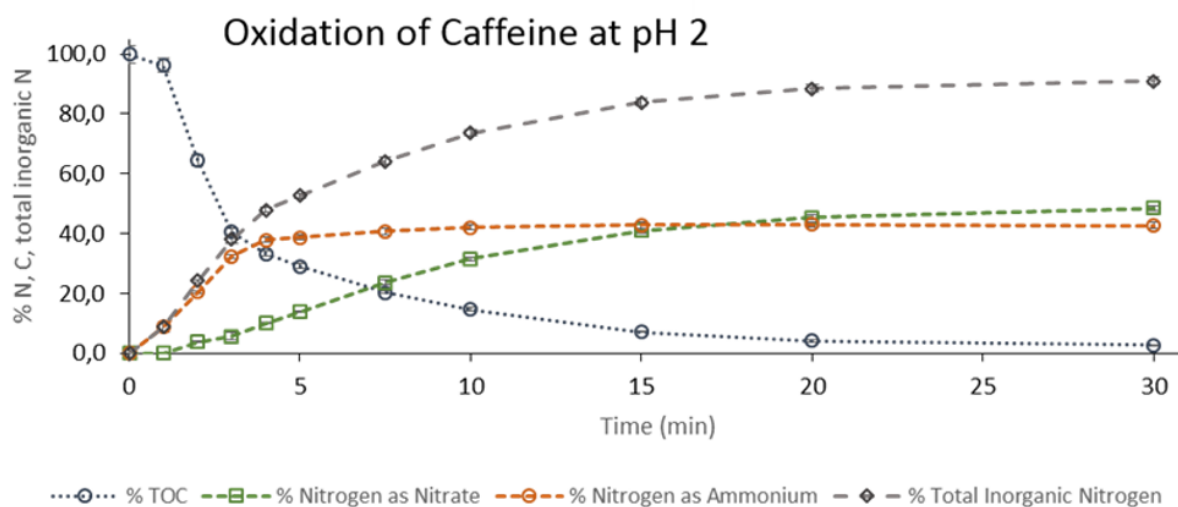
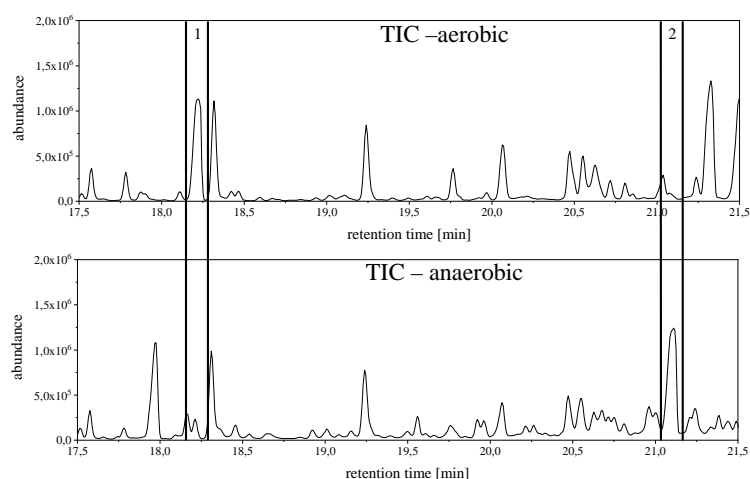


Figure 1 Mineralization of Caffeine by sulfate radicals under acidic conditions.

Characterization of the metabolome of *P. aeruginosa* in biofilms as a lung infection model**Involved staff:** Timo Köhler (AAC), PD Dr. Ursula Telgheder**Involved students:** Imke Ackermann, Laurin Domenic Grabler, Kübra Temel**Partners:** Prof. Dr. Oliver Schmitz, Applied Analytical Chemistry, University of Duisburg – Essen, Dr. Jost Wingender, Biofilm-Center, University of Duisburg – Essen**Funding:** German Research Foundation (DFG)

Example of the differentiation of growing conditions based on extracellular volatile metabolites. 1) 1-undecene is only detected under aerobic conditions and 2) 2-undecanone is exclusively formed under anaerobic conditions.

Cystic fibrosis (CF) is an autosomal recessive hereditary disease that leads to the production of thickened mucus in the infected organ (e.g. lung). Conditions in the infected lung favour polymicrobial infections, such as chronic lung infections with *Pseudomonas aeruginosa*. *P. aeruginosa* is the major pathogenic bacterium colonizing CF lungs at the end of the lifetime of CF patients. [A. Folkesson, Nat Rev Microbiol, 2012;10:841–51]

This *in vitro* study uses a biofilm model under conditions like those in a CF lung, including sampling of volatile extracellular metabolites, performed by a thin film microextraction (TFME) using polydimethylsiloxane films (PDMS). The analysis of the loaded films was performed by gas chromatography, coupled with a quadrupole mass spectrometer and thermal desorption (TD-GC-qMS). The method was successfully applied to standards of volatile metabolites known to be produced by *P. aeruginosa*. Detection and quantification limit for medium and less polar compounds using this method is in the lower nanomolar range (0.5 nM and 1.5 nM). A comparison with already published data from metabolome studies of the bacterium *P. aeruginosa* shows that this method can be used both for metabolic identification and for quantification in CF samples. The developed method was finally used to study the extracellular volatile metabolites of the strains *P. aeruginosa* DSM 50071, PAO1 and FRD1 under aerobic and anaerobic conditions. This study showed that different atmospheric conditions (aerobic and anaerobic) lead to the emission of different extracellular volatile metabolites. Different specific metabolites such as 1 undecene (aerobic; DSM 50071) and 2 undecanone (anaerobic; DSM 50071) could be identified.

In the future the *in vitro* biofilm model will be used to analyse the extracellular volatile metabolome of *P. aeruginosa* using artificial sputum and sputum medium, to get more closely to CF lung conditions.

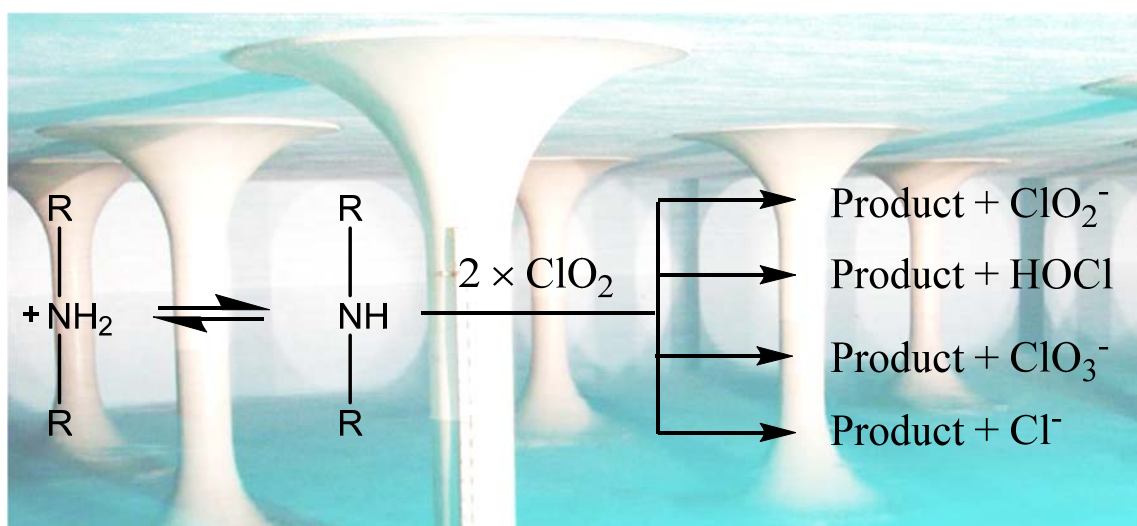
In addition, these findings enable the development of a non-invasive breath analysis method for CF patients with a focus on various bacterial infections.

Reactions of chlorine dioxide with nitrogen-containing compounds

Involved staff: Mohammad Sajjad Abdighahroudi, Dr. Holger V. Lutze, Prof. Dr. Torsten C. Schmidt

Involved student: Mischa Jütte

Funding: German Academic Exchange Service (DAAD) via the Federal Ministry for Education and Research (BMBF) Program "Sustainable Water Management"



Reaction of the disinfectant chlorine dioxide with nitrogen-containing compounds

Chlorine dioxide is used for the treatment of water for several decades. However, reaction mechanisms of pollutant degradation are hardly known. With the support of a DAAD scholarship, reactions of nitrogen-containing compounds with chlorine dioxide are investigated. Organic pollutants, though, are very complex and that aggravates their investigation. Hence, the present project focuses on the transferability of knowledge from model compounds to existing micropollutants. Simple model compounds such as N-heterocycles (e.g., piperidine, imidazole, etc.) will be used as surrogates for ritalinic acid, dexmedetomidine and other potential micropollutants that contain these moieties. In this regard, the following studies will be carried out for compounds: Reaction kinetics with ClO_2 and HOCl , yields of different chlorine products and stoichiometry

The project has shown that chlorine dioxide reacts fast with saturated N-heterocycles (amines) and rather slow with aromatic N-heterocycles. Since only deprotonated amines react with chlorine dioxide, the kinetics increases with pH. Two moles of chlorine dioxide are consumed per mole model compound transformed. In this reaction, chlorine dioxide gives rise to chlorite (electron transfer) and a radical cation. The radical cation may cleave H^+ and undergo an extremely fast second reaction with ClO_2 following different possible mechanisms. This behavior of chlorine dioxide was already observed by other researchers for aromatic compounds (e.g., phenol), and it was postulated that hypochlorous acid could be formed as the product of the second reaction. The results have shown that for saturated N-heterocycles, a second electron transfer reaction with the second nitrogen forms another chlorite. This was confirmed with more than 80% formation of chlorite as the primary ClO_2 transformation product. However, in the case of aromatic N-heterocycles (pyrrole and imidazole), the second attack did not form chlorite as its yield was only around 46% and 50%, respectively. The missing fraction of chlorine mass balance was indeed measured to be mostly HOCl , indicating an oxygen transfer reaction. The same behavior was also observed for micropollutants containing these moieties.

Theses completed in 2019

PhD Theses



21.02.2019

Fabian Itzel

“Investigation of agonistic and antagonistic endocrine activity during full-scale ozonation of waste water”

Summary

The use of a wide variety of chemicals in our society, such as industrial chemicals, pharmaceuticals, personal care products, etc., leads to pollution of surface waters. Especially in densely populated urban areas such as the Ruhr catchment, sustainable water management poses a major challenge. Despite intensive use through various types of discharges (effluents of direct dischargers, municipal waste water treatment plants, industry, etc.), good water quality has always to be guaranteed in accordance to the European Water Framework Directive. Endocrine disrupting chemicals can have an effect on aquatic organisms even at very low concentrations (pg/L range). In order to reduce the emission, ozonation was investigated as advanced waste water treatment for the elimination of organic trace compounds. An elimination performance of $\geq 80\%$ for selected substances at specific ozone doses in the range of $z_{spec.} = 0.3 - 0.7 \text{ mgO}_3/\text{mgDOC}$ was achieved. Since 2015, estrogens are listed on the watch-list of the European Water Framework Directive with required detection limits in the pg/L range. These detection limits cannot be achieved with current instrumental methods. Therefore, sensitive effect based methods based on modified yeast cells (*Arxula adenivorans*), which carry the human estrogen or androgen receptor, were used as a screening tool for corresponding activities. The results showed high elimination rates of the effects already at low ozone doses ($z_{spec.} = 0.3 \text{ mgO}_3/\text{mgDOC}$). Inhibitory effects (antagonists) were investigated in parallel. No significant reduction in antagonistic effects was observed. A comprehensive analysis method based on effect-based analysis and a non-target approach using high-resolution mass spectrometry was developed to identify unknown active compounds. Due to concerns about possible toxicity of the transformation products formed during the ozonation, biological post-treatments are recommended for further treatment. To characterize the efficiency of post-treatment, the assimilable organic carbon together with a trend analysis done by a non-target approach of unknown features formed during ozonation was established and demonstrated to be a useful tool.



12.04.2019

Laura Wiegand

“Characterization of reactive species in the Fenton reaction:
·OH vs. Fe^{IV}”

Summary

The term Fenton reaction describes the reaction of divalent iron (FeII) with hydrogen peroxide (H₂O₂) leading to formation of highly reactive species. Even though the reaction is known for more than 100 years, its mechanism is not fully resolved yet. In literature formation of an intermediate iron-peroxo-complex (Fe(H₂O₂)₂²⁺) is suggested, which is supposed to lead to formation of hydroxyl radicals (·OH) at acidic pH and to a tetravalent iron species (FeIV) at neutral or alkaline conditions. However, no experimental evidence for the formation of this intermediate could be found, yet. Elucidation of the Fenton mechanism is not only of scientific interest but also with regard to the use of the Fenton reaction in oxidative water treatment or pollutant degradation.

Accordingly, the present study aims to further elucidate the Fenton mechanism. For this purpose, the influence of various reaction conditions on existence, formation and stability of the postulated Fe(H₂O₂)₂²⁺-complex and resulting reactive products will be investigated. Additionally, the influence of different reaction conditions on the degradation of a model compound (bisphenol S) will be investigated. Finally, an alternative reaction leading to the formation of FeIV will be examined in order to investigate if FeIV is a relevant oxidant in the Fenton reaction.

This thesis presents the first kinetic indication for the existence of the postulated Fe(H₂O₂)₂²⁺-complex. Regardless of the FeII-concentration, at pH 3 the complex reveals constant stability, which is neither affected by the presence of an ·OH-scavenger. When the pH is increased from 1 to 4 decreasing decay rates of the intermediate are observed (ca. 70 s⁻¹ at pH 1 and 2 and ca. 50 s⁻¹ at pH 3 and 4). Furthermore, regardless of the pH determined ·OH-yields of ~100% based on the applied FeII-concentration did not reveal any indication for the formation of FeIV.

Examination of the pH-dependent influence of various organic chelating ligands indicates that even in the presence of these ligands an intermediate Fe(H₂O₂)₂²⁺-complex is formed, which forfeits stability with increasing pH. The quantification of ·OH-concentrations again does not reveal any indication of the formation of FeIV even in ligand-assisted Fenton reactions.

Investigations on the Fenton-based degradation of bisphenol S (BPS) shows that degradation can be influenced by applied reactant concentrations. However, it must be considered that too high concentrations of FeII and H₂O₂ may also cause ·OH-scavenging effects, which compete with degradation of contaminants. The optimum pH for BPS degradation was pH 3. Additionally, it could be shown that the Fenton-based degradation of contaminants in absence of ligands keeping FeIII dissolved is not restricted to acidic pH as it is hitherto assumed. Even at pH 7 BPS was completely

degraded. At pH values < 3, BPS degradation was observed to be restricted by insufficient Fe-recycling. The presence of •OH-consuming matrix components also limits BPS degradation. Comparative experiments dealing with the Fenton degradation of para-chlorobenzoic acid at pH 3 and 7, again did not show any indication for the formation of FeIV in the Fenton reaction, which could be involved in the degradation of the investigated pollutants.

The reaction described in literature for the generation of FeIV from FeII and ozone (O₃) could not be reproduced. Instead, the results suggest that FeIII is directly formed.

In summary, the first kinetic indication for the existence of the hitherto postulated intermediate Fe(H₂O₂)₂⁺-complex was obtained, which was observed to exclusively yield •OH at all reaction conditions investigated. Gained information can be used to make the application of the Fenton reaction more efficient in terms of wastewater treatment and remediation of contaminated sites. Nevertheless, further research is required to fully understand the whole Fenton process.



16.07.2019

Tobias Uber

“Adsorption and desorption processes on polymers in aquatic systems”

Summary

The sorption behaviour of high-density polyethylene (HDPE) and some other plastic materials in the aquatic environment with non-ionic organic compounds has already been studied to some degree although there is not yet a systematic approach to determine the sorption properties for a larger compound set. With the steady increase of interest on plastic materials in the environment, especially due to micro plastic particles (MP) or the great garbage patches, an increased demand for estimating sorption behaviours of those materials is mandatory. This is not only the case for HDPE but also for other plastic materials such as polystyrene (PS), lowdensity polyethylene (LDPE) or polyacrylate (PA). To this end, this thesis aims at a systematic investigation of sorption behaviour of selected plastic materials by use of probe sorbates in an aquatic environment. Sorption batch experiments with HDPE material used for water pipes and selected probe sorbates were carried out in a three-phase system (air/HDPE/water) covering an aqueous concentration range of at least three orders of magnitude. Sorption in the concentration range below 10⁻² of the aqueous solubility was found to be nonlinear and the Freundlich model was used to account for this non-linearity. Multiple regression analysis (MRA) using the determined distribution coefficients and literature-tabulated sorbate descriptors rendered robust ppLFFER models for all three concentration levels. Sorption was found to be dependent on polymer density and crystallinity by the ppLFFER model and the derived ppLFFER model described sorption more accurately than commonly used single-parameter predictions (spLFFER). A comparison of predicted data to experimental data from literature and this work demonstrated the strength of the ppLFFER, based on the training set over several orders of magnitude.

Batch experiments with PS were done with the same experimental approach but isotherms were evaluated with additional sorption models. The Freundlich fit rendered again the most robust data and it was shown that sorption of organic compounds to PS foil in water is nonlinear and that absorption is the dominant sorption mode. The properties directing the sorption to PS are impacted by non-specific and specific interactions. The specific interactions are driven mainly by the bipolarity/polarizability and it is shown to be influenced by the aromatic π - π -interactions of PS with the sorbates. As with other non-polar plastics, sorption is also driven by hydrophobic interactions.

A novel approach to determine distribution data is the inverse liquid chromatography (ILC) that was applied to HDPE. This is one of the first times the sorption behaviour of an environmentally relevant plastic material is investigated applying the ILC approach. The packed ILC columns rendered robust data that are comparable to data generated with the batch approach. The distribution coefficients from aged HDPE material were investigated under salty and salt-free conditions. The sorption strength for non-polar compounds did not change for aged HDPE compared to new HDPE material, whereas sorption for polar compounds did decrease significantly. Ionic strength of the eluent had a minor effect on sorption for both groups. The work showed that the ILC approach to investigate sorption properties under environmentally relevant conditions is promising and represents a feasible alternative to batch experiments. This thesis demonstrates that a systematic approach to determine sorption behavior with the help of probe sorbates renders robust results into molecular interactions with plastic materials in water. It also shows the benefit when using the ILC approach over the batch approach, in terms of easy variability of experimental conditions and time spent.



19.07.2019

Christian Becker

“Development of a Thermospray Nebulizer Interface for Liquid Chromatography with Flame Ionization Detection and Detector Response Studies of Volatile and non-Volatile Compounds”

Summary

Liquid chromatography (LC) is the analytical tool of choice for the investigation of by-products in pharmaceutical and chemical industry. The UV- and refractive index detector (RFID) encounter to the most common detectors for these purposes. The detection of unknown by-products deliver no sufficient information, since both detectors only can be used for a limited spectrum of analytes. Furthermore, without knowledge of the chemical structure, a semi-quantitative analysis is barely possible.

The flame ionization detector (FID) is advantageous to provide semi-quantitative data in the detection and quantification of, e.g., synthesis by-products in pharmaceuticals and chemical products. In contrast to commonly applied detectors, the FID signal is proportional to the carbon content of the analyte and allows the estimation of an analyte concentration directly out of the obtained signal. Several attempts to employ the FID for liquid chromatography have been carried out until yet [1].

This thesis described the development of a novel LC/FID interface and a FID response study of more than 100 compounds in order to achieve a better understanding of differences between gas chromatography (GC)/FID and LC/FID response data. The thesis was divided into 3 major sections: 1. a detailed study of previously described interfaces, 2. the development and optimization of a novel interface and 3. the analysis and comparison of response data obtained by GC/FID and LC/FID.

The historical conveyor type systems were designed to overcome the problems arise in FI detection by use of organic solvents in liquid chromatography. Therefore the systems dependent choice of non-volatile analytes in the beginning of LC/FID coupling change to volatile analytes by implementation of only water liquid chromatography [1]. Previously invented interfaces were studied to find out the advantages and disadvantages between the different types of interfaces, such as conveyor based interfaces, capillary jet interfaces or spray chamber interfaces. The focus was set on direct coupling techniques which can be operated without pre-evaporation steps of signal disturbing organic solvents, as known from conveyor type interfaces. The advantages and disadvantages of these interfaces were critically reviewed to design and present a novel interface.

In the development and optimization of the here designed interface the influence of the nebulizer material on flame stability and capillary blockage was shown. Previously reported problems such as blocking of the transfer capillary were solved using a stainless steel nebulizer body and transfer capillary. The effects of the working parameters such as backpressure, gas flow, distance between nebulizer nozzle and FID collector or FID temperature on the signal were analyzed.

The novel interface was validated for selected compounds known from literature. The linear correlation of the concentration and obtained FID signal of 21 N-heterocycles and 6 alcohols was found to be $R^2 = 0.991$ to 0.999 . The limits of detection of N-heterocycles ranged from 0.24 ng (pyrimidine-N-oxide) to 1.26 ng (s-triazin) absolute injected carbon. Obtained results for chromatographic separation of the alcohols propanol, butanol, pentanol and hexanol, used within previous studies in the field of LC/FID coupling were presented and compared to literature. The developed interface showed a substantial improvement of the absolute injected carbon concentration down to 0.28 ng (ethanol) in comparison to previously invented interfaces.

The use of different theoretical and practical response models was discussed to assist the response studies performed in the final section of the thesis. The scope was set on the experimental derived Effective Carbon Number (ECN_{Exp}) [2, 3] and experimental relative sensitivity (RF_{Exp}) [2, 4], respectively.

The influences of functional groups and substitutes, such as hydroxyl groups, halogens and ketones were discussed regarding former GC/FID studies. For some functional groups, effects on the obtained signals were found to be more negligible by extension of the carbon backbone. The influence of mono-alcohols decreased from C1 to C7. The effects of mono-, di- and poly-substituted compounds were compared and a substantial effect of the substitute location and the response factor was observed for, e.g., butan-1,2-ole.

Inflame processes for pyrimidine and pyridazine were proposed by the support of literature data. The response data of structural isomers obtained by theoretical response models (e.g. pyridine) were compared to experimental data of literature and within this study. The differences of theoretical

isomer response data (e.g. pyridine, pyrimidine) to experimental data were explained by the occurring inflame processes. In the end the response data were compared to GC/FID response data as far as they are available.

The present work is a great step forward for the analysis of volatile and non-volatile compounds using LC/FID. For the first time the responses of more the 100 different compounds were detected using LC/FID and compared to GC/FID response data if available. Much more LC feasible compounds are available, therefore further work is necessary to investigate all of this compounds and compare them to GC/FID responses. Further research in pharmaceutical industry is required to show the advantages of the semi-quantitative analysis of by-products by LC/FID.

Master Theses

Linda Hackl

„Entwicklung und Validierung einer LC-MS/MS Methode zur Bestimmung von Cyanobakterien-Toxinen in Oberflächengewässern“

(at Kooperationslabor RV/EGLV, Host supervisor: Dr. Christoph Haertel)

Frank Jacobs

„Entwicklung einer allgemeinen Methode zur Bestimmung des Substitutionsgrades unterschiedlich substituierter Cellulosederivate“

Mischa Jütte

„Oxidation of nitrogen-containing micropollutants with chlorine dioxide in surface water“

Michelle Klein

„Ecotoxicological impact of nitrogen-containing micropollutants and their oxidation products“

Riskyanti Lanyumba

„Analytical investigation of persistent microbubbles produced by pulsed laser ablation in liquid flow and their influence on the nanoparticle productivity“ (with Bilal Goekce, Technical Chemistry)

Valentina Merkus

„Analysis of transformation products during the ozonation of nitrogen containing compounds in presence of matrix constituents with LC-HRMS“

Paul Stark

„The aftermath of routine MRI diagnostics: Removal and recovery of gadolinium-based contrast agents by UV photolysis from urine of patients“

(at UFZ Leipzig, Host supervisor: Prof. Dr. Thorsten Reemtsma)

Bachelor Theses

Marina Braun

„Entwicklung eines Headspace-Kalibrierverfahrens auf der Basis von Silikonöl und nachfolgende GC-MS-Analyse“

Laurin Domenic Grabler

„Flüssigextraktion von TFME Folien und deren Anwendung für die Metabolomanalyse von P. aeruginosa aus dem Lungeninfektionsmodell mittels GCxGC-qMS“

Pascal Kadej

„Charakterisierung und Identifizierung von unbekannt organischen Spurenstoffen in Oberflächengewässern“

(at IWW Water Centre, Host supervisor: Dr. Peter Balsaa)

Miriam Patron

„Adsorbable organic halogen speciation method for wastewater“

(at University of Calgary, Host supervisor: Dr. Susana Kimura-Hara)

Lisa Szcesny

„Charakterisierung eines unbekannt organischen Spurenstoffs“
(at IWW Water Centre, Host supervisor: Dr. Peter Balsaa)

Lena Wykowski

„Analyse von semivolatilen organischen Komponenten in Olivenölen mit ITEX-DHS GC-MS“

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25. S. M. Schulte, D. Köster, M. A. Jochmann, R. U. Meckenstock:
Applying reverse stable isotope labeling analysis by mid-infrared laser spectroscopy to monitor BDOC in recycled wastewater
Sci. Tot. Environ. **665** (2019), 1064-1072
DOI: 10.1016/j.scitotenv.2019.02.061
26. T. Perl, N. Kunze-Szikszay, A. Braeuer, M. Quintel, A. L. Roehrig, K. Kerpen, U. Telgheder:
Aluminium release by coated and uncoated fluid-warming devices
Anaesthesia **74 (6)** (2019), 708-713
DOI:10.1111/anae.14601
27. N. Kunze-Szikszay, K. Walliser, J. Luther, B. Cambiaghi, V. Reupke, C. Dullin, W. Vautz, F. Bremmer, U. Telgheder, C. Zscheppank, M. Quintel, T. Perl:
Detecting Early Markers of Ventilator-Associated Pneumonia by Analysis of Exhaled Gas
Crit Care Med **47 (3)** (2019), e234–e240
DOI: 10.1097/CCM.0000000000003573

Conferences and Meetings

Organization



Annual Meeting of the Water Chemistry Society, Erfurt, May 27 to 29, 2019

(for more details check <https://www.wasserchemische-gesellschaft.de/de/erfurt-2019/seiten/wasser-2019>)



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Prof. Schmidt as president of the German Water Chemistry Society, Claudia Gehrke as secretary of the society and Dr. Lutze and his team of IAC members organized for the seventh time the annual meeting of the society, this year in Erfurt, Thuringia. After a year of heavy droughts in many parts of Germany, it was a rather obvious choice to devote the special topic of the conference on Tuesday afternoon to extreme events and their impact on water quantity and quality. The preceding public lecture on Monday night gave the topic a further historical perspective with insights on flooding events from 1500 to 2013. From IAC (current or past) Dr. Oliver Knoop, since April 2018 working as group leader at the TU Munich in the group of Prof. Drewes, presented results of his PhD thesis in Essen on toxicological effects of ozonation products of tamoxifen, and Gerrit Renner gave a presentation on his newly developed μ MAP process for fast mapping of microplastics on filters. Dr.-Ing. Asya Drenkova-Tuhtan, University of Stuttgart and Dr.-Ing. Maximilian Weissbach, formerly TU Munich were awarded with the Willy-Hager-Preis for their PhD theses "Phosphorus Elimination and Recovery from Wastewater with Reusable Nanocomposite Magnetic Particles" and "Technical implementation and development of

control strategies for the integration of the Coupled Aerobic-anoxic Nitrous Decomposition Operation (CANDO) into wastewater treatment schemes for simultaneous nitrogen removal and energy recovery from nitrogen”, respectively. The PhD prize of the Water Chemistry Society was also awarded twice to two outstanding young scientists, Dr. Tobias Bader, Langenauer Wasserversorgung, for his thesis "Mining of LC-HRMS data for the assessment of water treatment processes" and Dr. Jens Müller, Leibniz Institut für Ostseeforschung Warnemünde, for his thesis "Ocean Acidification in the Baltic Sea: Involved Processes, Metrology of pH in Brackish Waters, and Calcification under Fluctuating Conditions". Finally, Dr. Holger Lutze received the award of the Water Chemistry Society for his comprehensive scientific work on oxidative processes in aquatic systems and his long-lasting engagement for the Society.

8th Late Summer Workshop of the German Water Chemistry Society, Haltern am See, September 22 to 25, 2019

(for more details check <https://www.wasserchemische-gesellschaft.de/de/lsw-2019/seiten/lsw-2019>)



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The Late Summer Workshops have been established to provide an international forum for young scientists. The format is of the Gordon Research Conference type. The Late Summer Workshops of the German Water Chemistry Society have a long tradition and took place for the 8th time in 2019. Topics of the 2019 workshop were "Chemical and biological transformation processes and tools for their investigation". It was organised by the Water Chemistry Society and its Expert Committees "Oxidative processes", "Environmentally relevant transformation processes in the water cycle" and "Environmental isotope chemistry". Dr. Lutze was chairman of the scientific committee, Dr. Jochmann also a member, so IAC was well presented. meeting. Prof. Schmidt opened the workshop as president of the Water Chemistry Society. Main topics included structure elucidation, effects, transformation mechanisms, and regulation of chemical pollutants. Nine internationally renowned invited speakers set the stage and were involved in lively discussions with the 50 attendees who presented talks or posters.

Invited Lectures

T. C. Schmidt, L. L. Hohrenk, V. Hinnenkamp, P. Balsaa:
Suspect and Non-Target Screening in Water Monitoring: Three Recent Aspects under Scrutiny
SWEMSA 2019
Erding, October 23, 2019 (Invited Lecture)

T. C. Schmidt:
What shall we measure tomorrow? Needs and trends in future water analysis of organic micropollutants
BAM Analytical Colloquium
Berlin, April 04, 2019 (Invited Lecture)

T. C. Schmidt, L. L. Hohrenk, V. Hinnenkamp, P. Balsaa:
Suspect und Non-Target Screening in der Wasseranalytik
ANAKON 2019
Muenster, March 25, 2019 (Keynote Lecture)

T. C. Schmidt, P. Balsaa, A. Gottschlich, V. Hinnenkamp:
Kopplung von Non-Target-Analytik und toxikologischer Bewertung: Ergebnisse aus Oberflächenwasser- und Grundwasseruntersuchung
Essener Tagung 2019
Aachen, March 21, 2019 (Invited Lecture)

H. V. Lutze, T. C. Schmidt:
Removal techniques for perfluorinated compounds
30. Wassertechnisches Seminar (WTS)
Munich, February 13, 2019 (Invited Lecture)

U. Telgheder, T. C. Schmidt:
Anforderungen an Analyseverfahren für die Bestimmung von PFC in Umweltproben
Veranstaltung: PFC in Boden und Grundwasser: Erfassung, Untersuchung und Sanierung
B.E.W. – Bildungszentrum für Ver- und Entsorgungswirtschaft
Duisburg, December 04, 2019 (Invited Lecture)

Institute Colloquium

21.01.2019	Andrey Shevchenko, MPI of Molecular Cell Biology and Genetics, Dresden Shotgun lipidomics: analytical principles and biomedical applications
04.02.2019	Prof. Dr. Jean-Francois Focant, University of Liege, Belgium GCxGC coupled to TOFMS: A powerful tool for complex applications in Separation Science
20.05.19	Prof. Dr. Kevin Pagel, Free University Berlin Sugars in the Gas Phase – Novel Techniques to Unravel the Glycocode
03.06.19	Dr. Peter Boeker, University of Bonn Hochdurchsatz-Gaschromatographie mit negativem Temperaturgradienten: Messungen, Simulationen und Mehrdimensionalität
01.07.19	Prof. Dr. Philipp Weller, University of Applied Science Mannheim Authentizitätsanalyse mittels chemometrischer Verfahren
04.11.2019	Dr. Björn Meermann, BAM Berlin New ICP-(ToF)-MS based methods for material- and environmental analysis
18.11.2019	Prof. Dr. Uwe Karst, University of Muenster Hyphenated techniques to solve (bio)medical questions
04.12.2019	Prof. Dr. David Sedlak, University of California, Berkley Water Treatment for the Circular Economy

Teaching

At IAC we are involved in teaching mostly in the Bachelor and Master program “Water Science” that is a unique science-based curriculum with a focus on chemistry, analytics and microbiology (see details at <https://www.uni-due.de/water-science/>). All courses are also optional for students in the Bachelor and Master program “Chemistry”, some are also offered as elective courses for chemistry students studying towards a teacher’s degree and for students of the related Master programs “Environmental Toxicology” (offered in the faculty of biology) and “Management and Technology of Water and Wastewater – MTW3” (offered in the faculty of engineering).

Summer term

Lecture and Tutorial “Water Chemistry” (B.Sc. Water Science, in German)

Lecture “Water – The Lecture” (B.Sc. Water Science, in German)

Excursion to Wastewater Treatment Plant Duisburg-Kaßlerfeld (B.Sc. Water Science, in German)

Lecture and Tutorial “Oxidative Processes” (M.Sc. Water Science, in English)

Lecture and Tutorial “Stable Isotope Analysis” (M.Sc. Water Science, in English)

Laboratory Practical “Stable Isotope Analysis” (M.Sc. Water Science, in English)

Lecture and Tutorial “Quality Management” (M.Sc. Water Science, in English)

Laboratory Practical “Environmental Analytics” (M.Sc. Environmental Toxicology, in English)

Excursion to the Institute for Reference Materials and Measurements, Geel (B) (M.Sc. Water Science, in English)

Winter term

Lecture and Tutorial “Water Analysis” (B.Sc. Water Science, in German)

Laboratory Practical “Analytical Chemistry” (B.Sc. Water Science, in German)

Laboratory Practical “Water Chemistry and Analysis” (B.Sc. Water Science, in German)

Lecture and Tutorial “Water Chemistry” (M.Sc. Water Science and Environmental Toxicology, in English)

Lecture, Tutorial and Seminar “Chemometrics and Statistics” (M.Sc. Water Science, in English)

Individual Practical Projects “Analytical Chemistry” (M.Sc. Water Science, in English)

Excursion to the Drinking Water Treatment Plant incl. Ultrafiltration, Roetgen (M.Sc. Water Science, in English)

Outreach

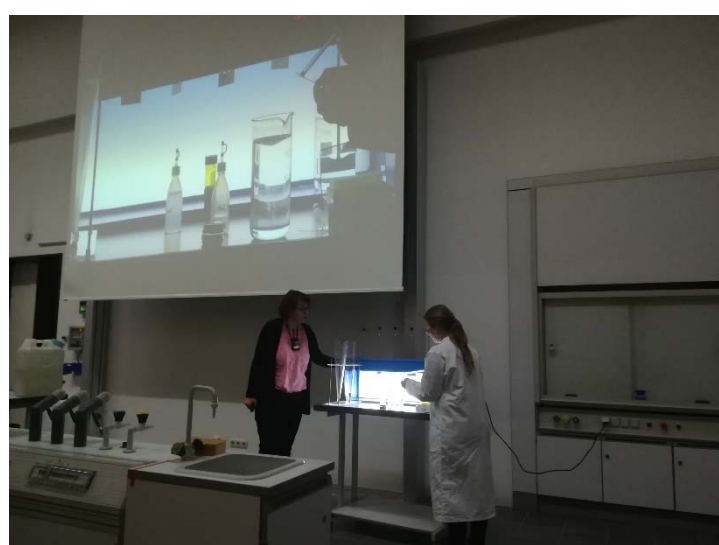
S.U.N.I SommerUni in Natur- & Ingenieurwissenschaften, 21. August 2018 „Der Blick ins Wasser“

S.U.N.I. is a unique platform for young people to support their study choice orientation in the natural and engineering sciences. By attending impressive experiments and presentations, the participants have the opportunity to experience the university's everyday life in special events and get to know the fields of work in science and technology in order to receive support for their study and career development process. The event "A glance at the water" includes sampling procedure at a small lake with subsequent analysis and water treatment of the samples in the lab. The participants learn fundamental strategies of chemical analysis and treatment techniques.



Trial Course of Studies (Probestudium Chemie), 17.12.2019 “Water Science – Zur Struktur des Wassermoleküls und den Folgen“

In addition to the early studies, pupils from upper classes have the opportunity to gain in-depth insights into the study areas of natural sciences, engineering and (economic) computer science, to speak with teachers, to explore the facilities of the University of Duisburg-Essen. Within the program of the Faculty of Chemistry, Dr. Ursula Telgheder, Dr. Klaus Kerpen, Max Reuschenbach and Lucie Tintrop presented an experimental lecture about the special properties of water. At first glance, the water molecule has a very simple structure. And yet it is something very special. Physicochemical: water is different as all structurally related compounds. That's why life, as we know it, makes it possible. Meaning: Water is involved in all biological and very many non-biological processes in our environment. It is an ideal solvent for many components, therefore the chemistry of and in aqueous systems is particularly diverse. The lecture went on from the special properties of water to water purification illustrated with simple experiments.



Miscellaneous

Births



Thomas Lutze, 18. Februar 2019



Jana Joksimoski, 19. Juni 2019



Nabila Ina Hohrenk, 18. Juni 2019

Weddings



Wiebke and Alex Kaziur-Cegla, 9. August 2019

Picture Galleries

Works Outing Trip to Gruga, Essen (September 06, 2019)

