

UNIVERSITÄT
DUISBURG
ESSEN



2018

Jahresbericht
Annual Report

Content

Instrumental Analytical Chemistry	2
Head of Chair	4
Secretarial Office	4
Regular Staff.....	4
Post Docs	4
Apprentices	4
Ph.D. Students.....	5
Internal	5
External.....	6
Research and Teaching Assistants.....	7
Guest Scientists	8
Awards.....	11
Running Projects at IAC 2018	14
Theses completed in 2018.....	35
PhD Theses	35
Master Theses	44
Bachelor Theses.....	44
Publications	45
Peer-reviewed Journals	45
Conferences and Meetings.....	48
Organization	48
Invited Lectures	51
Institute Colloquium.....	53
Teaching	54
Summer term	54
Winter term.....	54
Outreach.....	55
Miscellaneous.....	58
Picture Galleries	59

Instrumental Analytical Chemistry



Dear friends and colleagues,

as announced last year we indeed have been faster in compiling our annual report for 2018. Updates in a template are always easier than creating something new from scratch. Again, despite the considerable time spent on finalization it surely was worth the effort since sometimes only in retrospective you can really appreciate how many things happened throughout the year.

At least for me it was surely a special year due to my 50th birthday that I “officially” celebrated together with Oliver Schmitz as “100 years of Analytical Chemistry” in Essen but also with a party organized by all IAC colleagues on my birthday that really took me by surprise and will remain a very pleasant memory. Thank you all for this very special event! You can see a few impressions at the very end of this report.

Of course, we also worked hard throughout the year. As a result, we have published more papers in international journals than ever in my group’s history (27), including a virtual special issue for our graduate school Future Water published in *Science of the Total Environment* that I handled as managing guest editor.

Several new projects were granted and commenced in 2018 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.

Six PhD students finished successfully their thesis works and were awarded their doctoral degrees. Seven Master and six Bachelor students carried out their thesis at our department or at external partner institutes with a home supervisor at IAC. Dr. Andriy Kuklya left us after many years of successful scientific work in the ion mobility spectrometry group to take over a permanent position at the Federal Institute for Risk Assessment (BfR) in Berlin. We wish him all the best for his future!

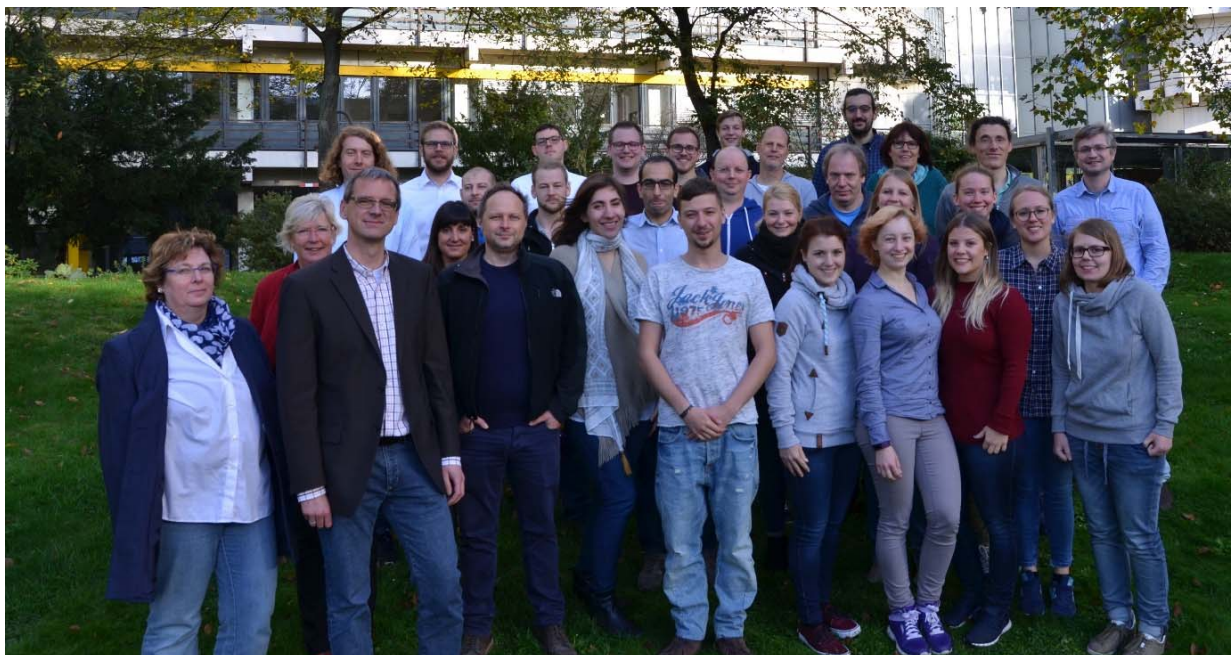
In addition to the annual meeting of the Water Chemistry Society in Papenburg in May, we have been involved in the organization of the 3rd and very successful MWAS in Mülheim in September.

Finally, I would like to thank 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 2019. We welcome very much feedback or collaboration interests for the future.



Torsten C. Schmidt



From left to right (front row): Lydia Vaaßen, Torsten Schmidt, Maik Jochmann, Mischa Jütte, Vanessa Wirzberger, Michelle Lüling, Wiebke Kaziur, Katharina Hupperich,

(second row) Claudia Ullrich, Rosangela Elliani, Nerea Lorenzo Parodi, Vanessa Hinnenkamp, Alexandra Fischbacher, Laura Wiegand, Lotta Hohrenk

(third row) Daniel Köster, Lokman Coban, Robert Marks, Sajjad Abdi, Florian Metzelder, Klaus Kerpen

(last row) Oliver Knoop, Nenad Stojanovic, Jens Terhalle, Frank Jacobs, Joel Geldermann, Robert Knierim, Sasho Joksimoski, Ursula Telgheder, Holger Lutze, Andriy Kuklya

Contact: Instrumental Analytical Chemistry
Department of Chemistry
University Duisburg-Essen
Universitätsstr. 5
45141 Essen

Phone: +49 201 183-6772/6774

Fax: +49 201 183-6773

email: torsten.schmidt@uni-due.de

www.uni-due.de/iac

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

Post Docs

Dr. Andriy Kuklya	Ion Mobility Spectrometry
-------------------	---------------------------

Apprentices

Christin Herrmann	Laboratory assistant
Tessa 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
Sasho Joksimoski	Novel coupling techniques for the determination of organic compounds in complex samples by ion mobility spectrometry
Alexandra Fischbacher	Formation and Quantification of ·OH in oxidative water treatment
Wiebke Kaziur	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)
Oliver Knoop	Formation and Effects of Transformation Products During the Ozonation of Tamoxifen
Xolelwa Lamani	Determination of aromatic amines as relevant toxicological components in aqueous and biological samples using comprehensive multi-dimensional GC-MS
Nerea Lorenzo Parodi	Aromatic amines as biomarkers in human urine: Analytical method development and epidemiological studies
Florian Metzelder	Investigation of sorption properties of carbon nanomaterials using packed columns and inverse liquid chromatography
Alyson Ribeiro	Ozonation and ecotoxicological assessment of two veterinary antibiotics: Cefapirin and Ceftiofur
Seyed Mohammad Seyed Khademi	Development of an on-line monitoring system for the analysis of organic contaminants in aquifers based on ion mobility spectrometry
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
Jens-Benjamin Wolbert	Characterization of glyphosate degradation by liquid chromatography-isotope ratio mass spectrometry (LC-IRMS)
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)
Frank Hitzgrath	Determination of diffusible hydrogen in high-strength steel related to lattice structure
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
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 Über	Adsorption and desorption processes on polymers in aquatic systems
Fabian Ude	Nicht-radioaktive, energetisch variable Ionisationseinheit zur Schadstoffanalyse in Baustoffen auf der Basis der FAIMS-Technologie
Tobias Werres	Microfluidic characterisation of high performance liquid chromatography systems with the main emphasis on the intrinsic efficiency

Research and Teaching Assistants

Katharina Hupperich

Frank Jacobs

Mischa Jütte

Pascal Kaiser

Hyerin Kim

Valentina Merkus

Simon Nikutta

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



M. Sc. Rosangela Elliani, University of Calabria, Arcavacata di Rende, Italy

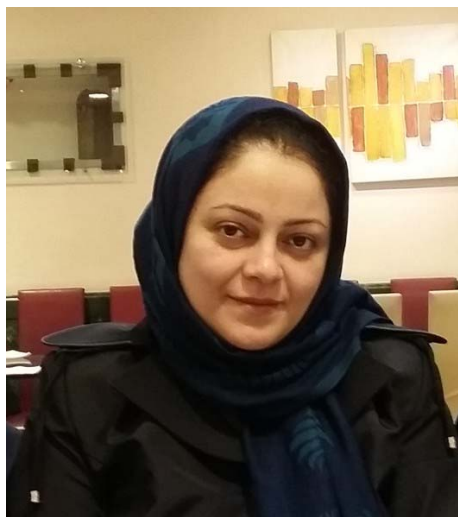
The analysis of Fatty Acids (FA) and their Methyl Esters derivatives (FAMES) has become a topic of great importance in the last years, reaching a great variety of different fields. Despite the increased number of FAMES-related publications, there is no report yet on the use of the novel SPME Arrow approach for their analysis. Therefore, a comprehensive comparison of different SPME fibers and SPME arrows for the analysis of a 37 component FAMES mix was accomplished.



Prof. Akinsehina Akinlua, Obafemi Awolowo University, Ile-Ife, Nigeria

The project was on the development of green analytical protocol for the determination of diamondoids content of petroleum source rock. The study investigated the use of benign non-ionic surfactant as the extraction solvent. A three-level full factorial design of experiment (DoE) was employed for the development of the method, involving three main variables; concentration of solvent, extraction temperature, and extraction time. All the experiments were performed with the aid of accelerated reaction microwave. In-tube microextraction using TENAX TA as sorbent in combination with GC-MS was used to profile the diamondoids in the extract. The findings revealed that the three variables have significant effects on extraction yields of the diamondoids. The yields of the analytes at the optimum conditions of the new

method were better than those from the existing method.



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

The main aim of the academic visit, was initiation of a collaboration with Prof. Torsten C. Schmidt and his scientific staff in the field of environmental screening. To that end, multivariate chemometrics methods have been employed for comprehensive data evaluation of liquid chromatography coupled with high resolution mass spectrometry (LC-HRMS) system. Both target and nontarget screening of organic micropollutants (OMPs) in drinking and wastewater samples was performed in this visit. The main contribution in this project was conducted by Lotta Hohrenk (PhD student).

The combination of the data compression and multivariate curve resolution strategy performed in this study allowed to overcome most of the encountered challenges, such as efficient data size reduction, alignment-free tracing of pollutants, tackling spectral interferences and highly overlapped OMPs elution profiles through one two-way decomposition step, feature prioritization and tentative identification of discriminatory pollutants between different classes of water samples.



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

In this academic visit, a collaboration with Prof. Torsten C. Schmidt and his scientific staff was accomplished. An automated PAL SPME Arrow technique coupled with GC-MS was developed, optimized and evaluated for determination of T&O compounds in water samples. Sensitivity of the developed method was satisfactorily high to produce statistically significant quantitative results below the odor threshold of the examined T&O compounds. Analytical performance characteristics of the optimized PAL SMPE Arrow

in demonstrated a fast, straightforward, reliable, robust, precise and accurate technique, which can be implemented for analysis of the lowest practically relevant concentrations of T&O compounds in surface water samples.

Awards



© Picture: Laborpraxis

Mohammad Sajjad Abdighahroudi
Metrohm Young Chemist Award (10.04.2018)

In this research, an ion chromatography method has been investigated to determine the free chlorine in water by using glycine as probe compound. The amine group of glycine can readily scavenge free chlorine and form *N*-chloroglycine. Due to chlorination, pK_a value of the amine and carboxylic group will be lowered and the anionic species of *N*-chloroglycine will be the predominant species in a wide range of pH and thus can be determined by IC. Meanwhile, the *N*-chloroglycine can oxidize iodide to triiodide and cause a strong response in an iodometric post-column reaction with UV detection. This method allows for a selective and sensitive measurement of hypochlorous acid.



Lucie Katharina Tintrop: „Grundlegende Untersuchungen zu der Ozonung von verschiedenen Phenolderivaten“ (2. Axel Semrau Award, 17.12.2018)

In this research Luci Tintrop investigated fundamental reactions of ozone with different phenol derivatives. She focused on the formation of highly reactive species such as hydroxyl radicals and on reaction stoichiometry. These results were used to develop new aspects of the reaction mechanism of ozone with phenols. Since phenolic moieties are present in pollutants and in natural organic matter, her work improves the overall understanding of ozone based water treatment processes.



Yanina Müller (2nd from the right): „Identification and Quantification of microplastics in the longitudinal profile of the river elbe, Germany” (1st Venator Water Award, 17.12.2018)

Micro-plastics is a new research area in the field of environmental research. Sources of micro-plastics are manifold e.g., abrasive materials in washing agents or deteriorated plastic waste. Recent research indicates that micro-plastic may be ubiquitous, however exact information on the amount and kind of micro-plastic in the aquatic environment is largely unknown. This knowledge is mandatory for assessing impacts of micro-plastic on health and the environment. Yanina Müller investigated the occurrence of microplastic in the river Elbe.

Lotta Laura Hohrenk (2nd from the left): "Development and validation of a suspect-target method for the screening of micropollutants and transformation products in the aquatic environment" (Venator Water Award, 17.12.2018)

Lotta Hohrenk developed a non-target-screening method with a set of model analytes on a LC-HRMS system. Thereby, she investigated detection limits, matrix effects, mass accuracy and reproducibility of retention times and peak areas. The non-target analysis is an innovative approach to characterize aquatic environmental or technical systems. The method allows to monitor e.g. pollutant entries and may help establishing early warning systems.



Hyerin Kim (at the right)

On 17.12.2018 Hyerin Kim was awarded for best performance in analytical chemistry during the curriculum Water-Science (Master) by Mikheil Gogiashvili (GDCh, Division of Analytical Chemistry).



Lotta Laura Hohrenk (2nd from the right)

Young Scientist Award 2018, Centre for Water and Environmental Research (ZWU) for her master thesis "Development and validation of a suspect-target method for the screening of micropollutants and transformation products in the aquatic Environment" (12.07.2018)

Running Projects at IAC 2018

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 Associate PhD student), Dr. Holger V. Lutze, Claudia Freimuth (Coordinator), Prof. Dr. Torsten C. Schmidt (Speaker)

Involved students: Valentina Merkus

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”



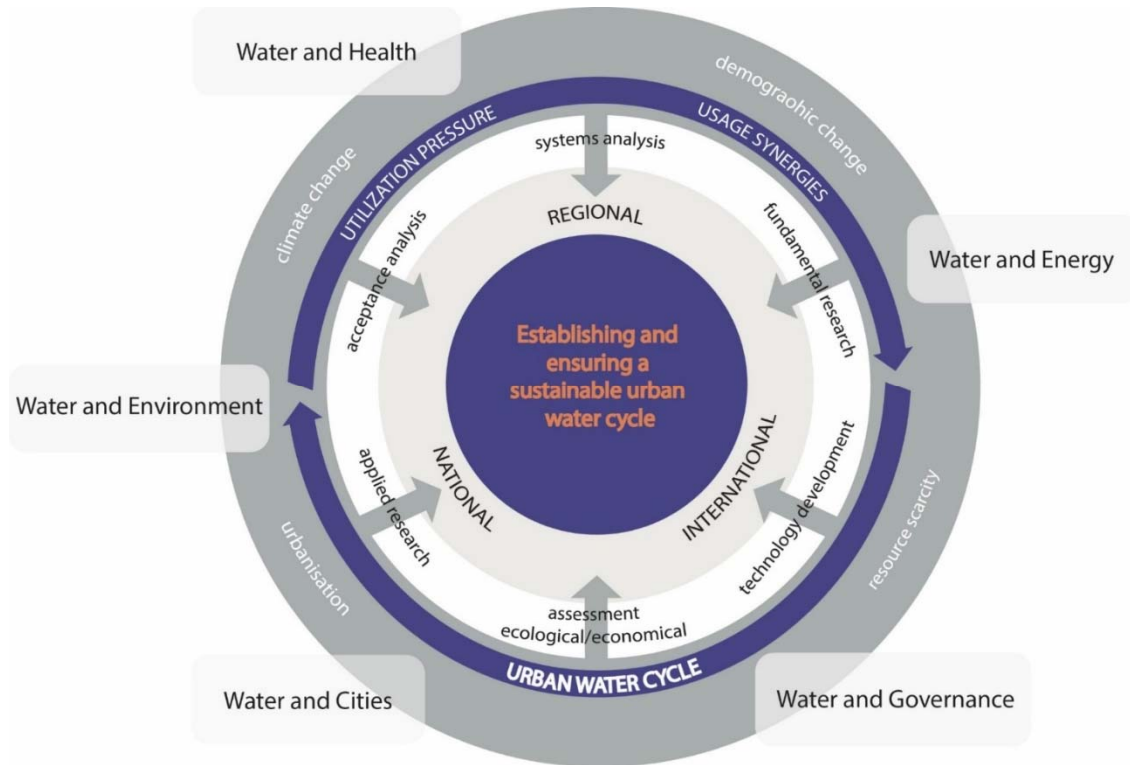
The multiperspectivity of inter- and transdisciplinary approaches allows to conduct innovative and path-breaking research. Combining knowledge and methods across disciplines makes possible to identify hitherto unnoted research questions. Tackling questions from different and novel angles allows to find 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 during ozonation with special focus on the reaction with matrix components and the formation of transformation products and their toxicity to aquatic organism.



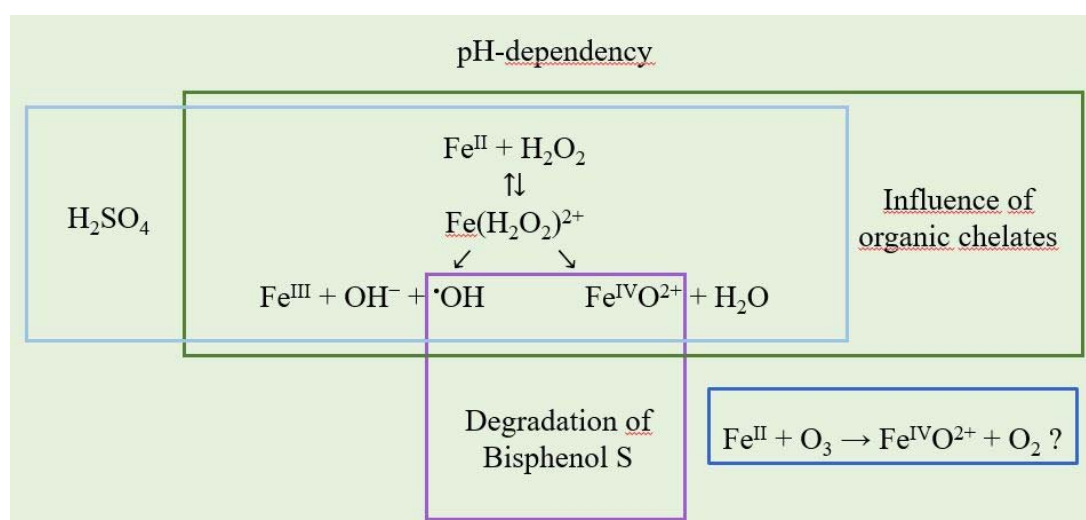
Characterisation of reactive species in the Fenton reaction ($\text{Fe}^{\text{II}} + \text{H}_2\text{O}_2$) - $\cdot\text{OH}$ vs. Fe^{IV} (Fenton II)

Involved staff: Hanna Laura Wiegand, Dr. Holger V. Lutze, Dr. Klaus Kerpen, Prof. Dr. Torsten C. Schmidt

Involved students: Timon Orths, Katharina Hupperich, Mischa Jütte, Anke Dinter

Partners: Prof. Dr. Clemens von Sonntag (deceased)

Funding: German Research Foundation (DFG)



For a better understanding of mechanistic aspects of the Fenton reaction ($\text{Fe}^{\text{II}} + \text{H}_2\text{O}_2$) the influence of pH and presence of various organic chelates at pH 2 – 6 has been investigated with respect to existence and lifetime of an intermediate $\text{Fe}(\text{H}_2\text{O}_2)^{2+}$ -complex and corresponding $\cdot\text{OH}$ -yields in the Fenton reaction. It was found that the postulated intermediate $\text{Fe}(\text{H}_2\text{O}_2)^{2+}$ is generated and quantitatively transformed into $\cdot\text{OH}$, OH^- , and Fe^{III} ($\sim 100\%$ $\cdot\text{OH}$ -yields per $[\text{Fe}^{\text{II}}]_0$) regardless of pH and type of chelate. This may allow to use the Fenton reaction for remediation or as part of industrial wastewater treatment in absence of organic chelates at pH 1 – 4 as well as in presence of those ligands at pH 2 – 6. Formation of Fe^{IV} as a rather mild oxidant would largely limit the range of pollutants, which could be degraded. Furthermore, real water matrix constituents may serve as complexing agents similar to the investigated chelates.

In summary, results obtained in WPs 1, 3, 4 and 5 did not indicate appreciable formation of Fe^{IV} . Indeed, only an indirect approach was applied to rule out Fe^{IV} -formation in Fenton experiments but nevertheless, in case of considerable formation of Fe^{IV} in these reactions, $\cdot\text{OH}$ -yields must have been markedly lower than 100 % per $[\text{Fe}^{\text{II}}]_0$. However, it is still possible that at reaction conditions not assessed in the course of this project Fe^{IV} might become relevant.

After those mechanistic investigations applicability of the Fenton reaction in terms of contaminant degradation was examined using bisphenol S (BPS) as model compound. It could be shown that degradation efficiency strongly depends on different parameters such as the ratio of $[\text{H}_2\text{O}_2]$ to $[\text{Fe}^{\text{II}}]_0$ or pH. With respect to the application of Fenton's reagent for degradation of contaminants in real samples these parameters must be adjusted considering actual conditions. Furthermore, it must be balanced between degradation time and chemical demand.

Wastewater treatment on basis of chlorine dioxide (ABC)

Involved staff: Dr. Holger V. Lutze, Jens Terhalle, Prof. Dr. Torsten C. Schmidt

Involved students: Mischa Jütte, Johanna Buss

Partners: a.p.f. Aqua System AG

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



Chlorine dioxide pilot plant

This project deals with the application of chlorine dioxide for degradation of micropollutants in wastewater.

Wastewater treatment plants are an important source for micropollutants in the aquatic environment. Hence, for mitigating micropollutants wastewater treatment plants are currently retrofitted with advanced treatment steps based on activated carbon or ozone. Both steps have a similar efficiency in removing micropollutants from wastewater. In contrast to activated carbon, ozonation can also partially disinfect wastewater. However, ozonation also results in formation of undesired products such as cancerogenic bromate (US-EPA drinking water standard $10 \mu\text{g L}^{-1}$). Chlorine dioxide is also a strong oxidant, which does not form bromate and may thus be an alternative process to wastewater ozonation.

The project has shown that pollutants with activated aromatic moieties (e.g., ethinylestradiol, sulfamethoxazole, diclofenac) can be readily degraded by chlorine dioxide. Interestingly, a degradation of some compounds, which barely react with chlorine dioxide, was also observed (e.g., atenolol). This was explained by the formation of the secondary oxidant hypochlorous acid, which reacts fast with atenolol. However, ozonation still appeared to degrade a larger range of micropollutants than chlorine dioxide. As by-product chlorine dioxide forms chlorite (US-EPA drinking water standard 1mg L^{-1}). Yet, the relevance of chlorite formation in wastewater treatment is investigated.

First results of the present project also indicated that chlorine dioxide may be a very good disinfectant. Currently, importance of wastewater disinfection increases since antibiotic resistant microorganisms in the environment were observed.

Results from bench scale were successfully up-scaled to pilot scale at a real wastewater treatment plant, indicating that a full-scale application of chlorine dioxide in wastewater treatment may be possible.

Treatment of Tai Hu water

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

Involved students: Mischa Jütte, Pascal Kaiser, Johanna Buss, Robert Marks

Funding: Federal Ministry of Education and Research (BMBF)

Under contract of Research Centre Jülich (Dr. Stephan Küppers)

Close cooperation with Inge GmbH (Christian Staaks), bbe Moldaenke GmbH (Christian Moldaenke), TZW Dresden (Dr. Wido Schmidt) and institute of mechanical engineering (University Duisburg-Essen, Prof. Panglisch, Sucipta Laksonon, M. Sc.), IWW Water Centre (Dr. Tim aus der Beek, Dr. Andreas Nahrstedt)



Aerial image of Tai Hu Lake and ozone depletion after flocculation and membrane filtration (bench scale experiments)

The Tai Hu (Tai Lake) is used as a raw water reservoir for approximately 10 million inhabitants predominantly in the Jiangsu province, China. Algae/cyanobacterial blooms occur frequently in the eutrophic shallow lake and represent a challenge for drinking water treatment. Furthermore, occasionally taste & odor (T&O) problems have been reported in drinking water. Due to the impact of wastewater and surface water runoff, also presence of pesticides and emerging pollutants such as pharmaceutical compounds have to be considered.

It was shown, that part of the T&O compounds present in finished drinking water are formed from reactions of amino acids during water treatment (e.g., by chlorination). These amino acids may be part of the algae organic matter that may be released after cell lysis in conventional water treatment using pre-ozonation, flocculation and sedimentation. Our results have shown that ozonation can cause lysis of algae with subsequent release of intracellular material. Hence ozonation should be performed after a filtration step. The process consisting of 1. flocculation, 2. ultrafiltration and 3. ozonation was investigated in a combination of pilot- and bench scale experiments. The results revealed that the pretreatment by flocculation and ultrafiltration does not only remove intact algae cells but also improves the overall performance of the ozonation step. The combination of flocculation and ultrafiltration removes a part of the dissolved organic matter which reduces the required ozone dose. First results have also shown, that direct ozonation of the Tai Hu water may be prone to form halogenated organic compounds. This was deduced from the observation that after addition of ozone

bromide was oxidized, while the final product bromate (undesired disinfection by-product with a US-EPA and EU drinking water standard of $10 \mu\text{g L}^{-1}$) was formed to a minor extent (incomplete bromine mass balance). The remaining fraction of oxidized bromide (e.g., hypobromous acid) might have reacted with organic matter to form brominated organic compounds. After flocculation and ultrafiltration though, bromide recoveries (sum of bromide and bromate) very much improved. It is worth mentioning that halogenated organic compounds may also originate from chlorinated wastewater discharge into the Tai Hu.

The formation of halogenated products and strategies for bromate minimization are currently investigated. Furthermore, the treatment chain shown above will be investigated in pilot scale with additional bench scale experiments.

Water and wastewater ozonation feasibility studies

Involved staff: Dr. Holger V. Lutze

Involved students: Mischa Jütte, Pascal Kaiser, Robert Marks

Funding: Partners from water industry

Cooperation with IWW Water Centre (Marcel Koti, Anil Gaba, Dieter Stetter, Andreas Nahrstedt) and IUTA (Andrea Börgers, Jochen Türk)



Generator for ozone stock solution

In cooperation with IWW and IUTA several feasibility studies on wastewater ozonation were performed. One important factor in water treatment is energy demand, which can represent a large part of the operational costs. One strategy to reduce costs is a dynamic treatment performance taking fluctuations of electricity prizes into account (.e.g., reduced treatment performance at high costs for electricity and vice versa). Such kind of concepts were investigated in the project Enerwa. A part of the work dealt with energy saving strategies for ozonation, which were investigated in pilot scale and bench scale experiments.

Ozonation is also applied in wastewater treatment for removal of residual anthropogenic trace compounds. Since, trace compound removal in wastewater treatment was supported by government in NRW many operators of wastewater treatment plant engaged bench scale studies in wastewater ozonation to assess the operational conditions for a full scale ozonation plants. These bench scale experiments investigated the amount of ozone needed for degradation of pollutants as well as the required hydraulic retention time of the ozonation reaction tanks. In wastewater ozonation higher ozone dosages have to be applied. This is mainly due to the concentration of organic matter (OM) in wastewater (average app. 5 – 10 mg L⁻¹ OM) which is higher compared to source water used for drinking water purification (average app. 0.5 - 2 mg L⁻¹ OM).

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).

The objectives of the targeted research in the planned collaborative project are as following:

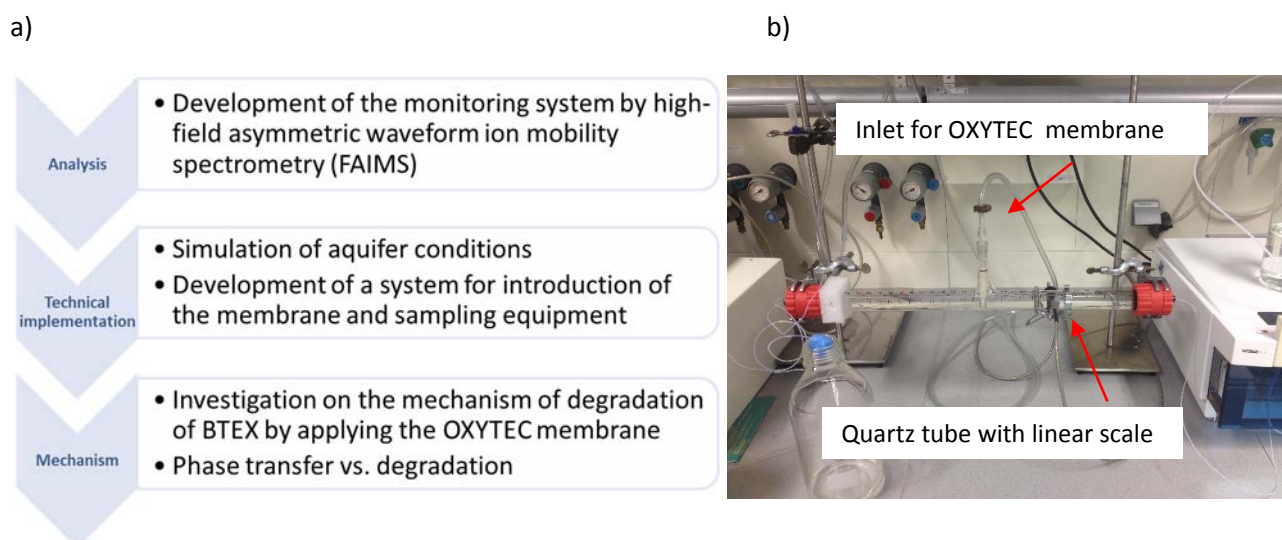
- 1- Developing smart chemometrics-assisted strategy coupling of LC-HRMS with multivariate modelling algorithms.
- 2- Exploiting multivariate advantage for quantification of environmental contaminants.
- 3- Facilitating non-target screening using LC-HRMS for identification of a higher number of contaminants in water using multivariate curve resolution and pattern recognition methods: assessment of a wastewater treatment plant effluent and diffuse sources of pollution such as run-off from roads and agricultural fields as a case study by simultaneous multivariate analysis of LC-HRMS data matrices.
- 4- Comparison of data generated for samples from Germany and Iran with regard to water pollution caused by various emission sources by exploiting statistical classification methods.

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

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

Partners: Fabricius Pro Terra GmbH

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



(a) Overview of the scientific issue (b) Monitoring of the Fe-oxidation

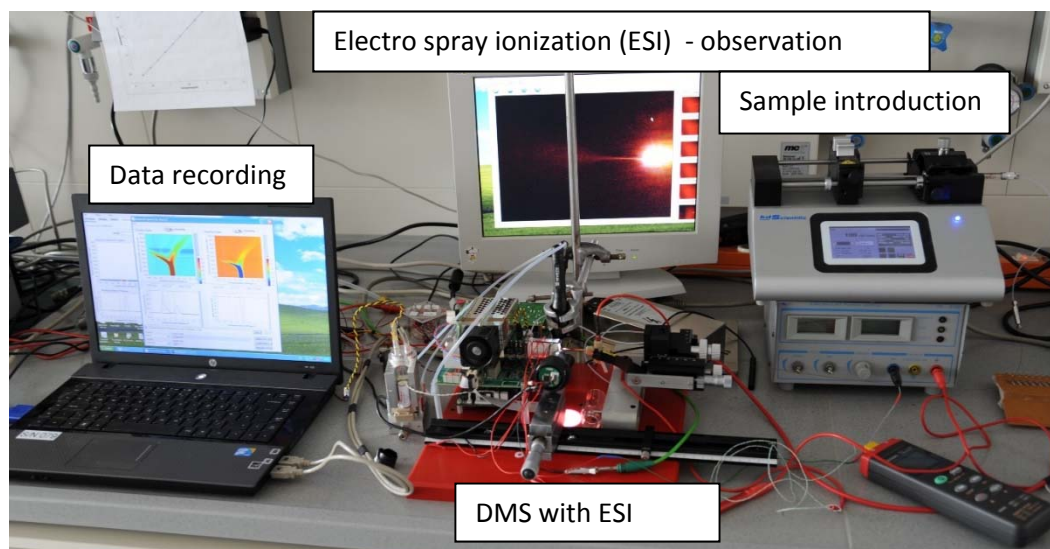
The company site of a chemical industry in Ruhr area was acquired as a test site for the testing of the combined in-situ and monitoring process for the treatment of groundwater. In the 1960s, there was a significant amount of benzene, toluene, ethylbenzene and xylenes (BTEX) due to a defective line. Since the late 1970s, the unsaturated soil zone has been remediated by means of soil air extraction (pressure 0.2 and 0.6 bar), which cleans the groundwater and soil air carried in. The soil air is removed from the condensate and further purified by means of activated carbon. Samples from this industrial site will be used for simulation of aquifer conditions. Oxygen will be introduced by the OXYTEC membrane. The hypothesis is that degradation of BTEX takes place by microorganisms in anaerobic (reductive) conditions. For the growing of those microorganisms a certain amount of Fe^{3+} is necessary which will be provided by the oxidation of Fe^{2+} by the added oxygen.

Fast on-site analysis for the detection of pesticides in water by 2D-DMS (Hydro-2D-DMS)

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

Partners: Ampegon PPT GmbH

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



Laboratory set up of a DMS with electro spray ionization

The aim of this project is the development of a sensitive, cost-effective analytical system for monitoring of selected pesticides (quinoxifen, cybutryne, dichlorvos, terbutryn) in different water matrices with regard to the legally binding limit values. The analytical system is based on differential mobility spectrometry (DMS) technique. Commercially available DMS-systems are limited to fixed frequencies (1MHz) of the electrical field. In the frame of this project, a detector will be developed with variable frequencies in order to enlarge the detectable range of masses with high sensitivity.

In a first step, a home made electrospray ionization (ESI) source was coupled to a commercially available DMS in a laboratory setup. The analysis of aqueous solutions of benzene, toluene, ethylbenzene, p-xylene and naphthalene with the ESI source as ionization unit in combination with a commercial DMS showed that the water separation of the analyte ions was insufficient. The strongly solvated ions significantly reduced the signal intensity. Therefore, a desolvation unit is necessary. Alternatively, a photoionization lamp will be used for the ionization of the analytes.

The detector comprises the following functional assemblies: The (1) gas inlet, the (2) ionization section, the (3) excitation, the (4) measuring cell, the (5) gas outlet and a (6) heating. As a geometric building structure, a two-plate geometry with a flat, rectangular flow cross-section was chosen.

All functional assemblies are arranged longitudinally and built into this two-plate geometry. As assemblies serve copper-laminated boards with defined layers, which are integrated in an electrically conductive frame made of aluminum. This frame will also serve as a holder for the UV lamp (ionization) and for heating. As a spacer of the boards Kapton films are used, which define both as insulators of the boards as well as the height and width of the flow channel.

Development of a Direct Inlet Probe - Atmospheric Pressure Photoionization – Ion Mobility Spectrometers (DIP-APPI-IMS) -system for quality control of chemical and pharmaceutical products (DIPPI-IMS); Development of a miniaturized IMS coupled to direct inlet probe (DIP)

Involved staff: Dr. Andriy Kuklya, PD Dr. Ursula Telgheder

Partners: SIM GmbH

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



Structure of APPI-DIP-IMS: 1: DIP; 2: IMS; 3: heatable dopant feed; 4: power supply and control module for APPI-IMS; 5 and 6: power supply and control module for DIP; 7: transimpedance amplifier; 8: measurement data acquisition module; 9: Calculator (shows typical drift spectrum)

The aim of the project was to provide a sensitive, cost-effective and fast process for product and quality control in various industries, such as chemical and pharmaceutical industries.

For this purpose, a DIP-APPI-IMS system was successfully developed and manufactured. It consists of a miniaturized and automatable sample loading system (Direct Inlet Probe, DIP) and a miniaturized ion mobility spectrometer (IMS). The DIP unit allows the direct introduction and temperature-controlled evaporation of solid and liquid analytes. The analytes are ionized after evaporation by means of photoionization at atmospheric pressure (APPI) and separated within a few milliseconds (<10 ms) in the miniaturized IMS system.

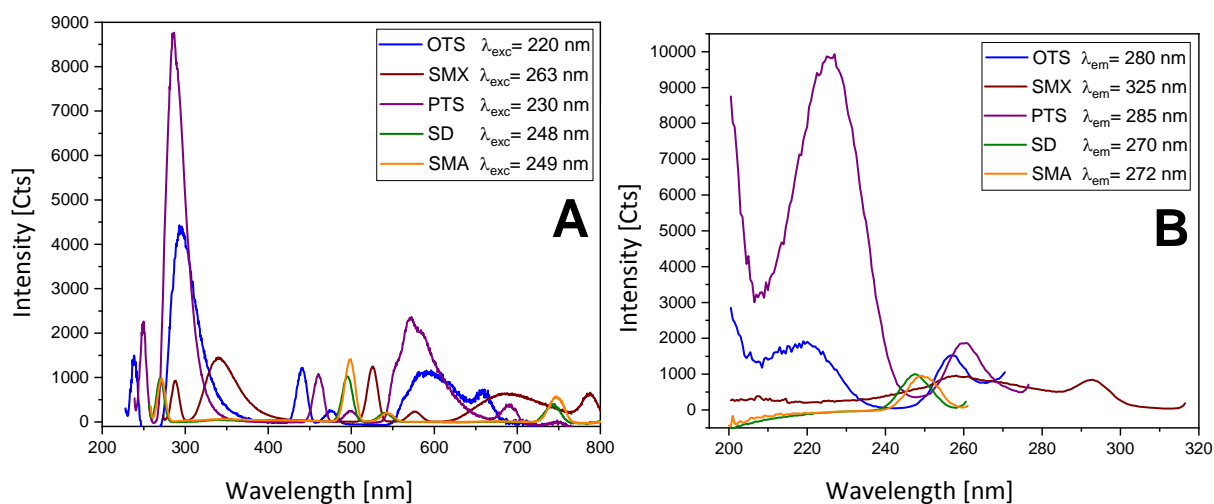
However, the list of model substances has been modified. In addition to active substances such as sulfamethoxazole and bisphenol A, the environmentally relevant polycyclic aromatic hydrocarbons were also analyzed. Due to the ongoing equipment optimization work, no real samples have been analyzed with DIP-APPI-IMS.

Fast on-site-detection of sulfonamides in ground- and surface water by 2D-fluorescence spectroscopy (MultiDimSpec)

Involved staff: Dr. Klaus Kerpen, PD Dr. Ursula Telgheder

Partners: GO Systemelektronik GmbH

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



Emission spectra (A) and excitation spectra (B) of aqueous solutions (1 mg / L) of paratoluenesulfonamide (pTs), ortho-toluenesulfonamide (oTs), sulfadiazine (SD), sulfamethazine (SMA) and sulfamethoxazole (SMX)

The aim of the project was the development of a miniaturized system, which allows a fast on-site analysis of selected sulfonamides in waters with different matrix components, taking into account the legally required orientation values. As a detection method, 2D fluorescence spectroscopy was used, because due to the intense fluorescence of the sulfonamides, the sensitivity is high enough to be able to determine the concentrations required as orientation values. The necessary selectivity was achieved by recording and data analysis of the emission spectra at different excitation wavelengths.

In addition to the antibiotic sulfamethoxazole (SMX), which is frequently detected in the aquatic environment, p-toluenesulfonamide (pTs), o-toluenesulfonamide (oTs), benzenesulfonamide (BS), sulfadiazine (SD) and sulfamethazine (SMA) were selected as further indicator substances. The prototype tested in laboratory tests was integrated into a multi-sensor system. In addition to the control software, complex software modules had to be created for the data evaluation.

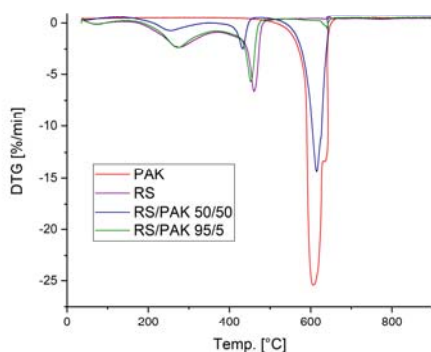
“Den Spurenstoffen auf der Spur – Teil 3” (DSADS)

Involved staff: PD Dr. Ursula Telgheder

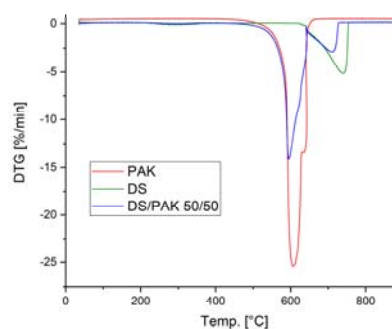
Involved students: Anna Lena Röhrig

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 1 (RS) / Activated carbon powder (PAK))



Differential mass loss thermograms of thermal decomposition of Dry substances (Return sludge 2 (DS) / Activated carbon powder (PAK))

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.

Using thermogravimetry in combination with differential thermoanalyses the determination of activated carbon in presence of natural organic matters has been investigated. The mass losses of pure dried substance released from two different treatment plants and from the activated carbon as well as the mass losses of defined mixtures of both compounds were determined. As it is shown in the figures above the mass losses of the different substances took place at different temperatures.

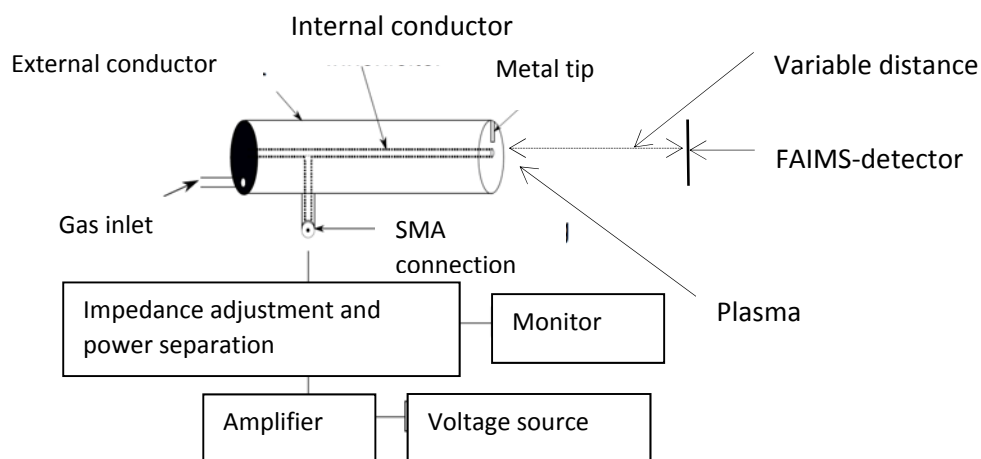
Therefore, future work relates to the optimization of the experimental parameters, e.g. use of nitrogen for the pyrolysis of the volatile organic substances, heating and gas flow rate. Furthermore, the limit of detection and limit of quantification of the method should be determined on the basis of the calibration.

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, Robert Marks, PD Dr. Ursula Telgheder

Partners: Schumann Analytics GmbH

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



Design of the innovative ionization unit

The aim of this project is to develop a non-radioactive, energetically variable ionization unit which, 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). At the same time, the substances should be reliably detected both qualitatively and quantitatively. As model substances pentachlorophenol, lindane, tolylfluanid, propiconazole and formaldehyde are selected. The development of a suitable sample preparation and calibration method is also the focus of the requested project. With the device being developed, manufacturers of new construction products will have a system in place to check product emissions as part of ongoing process control and factory conditions. By using the developed technique, the production process can be influenced very quickly to control the pollutant emission and eventually reduce it.

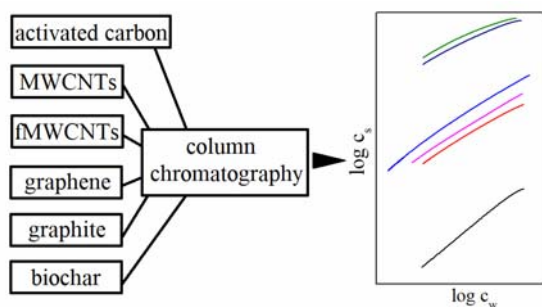
Characterization of sorption of non-ionic organic compounds on carbon-based nanomaterials (Sorption II)

Involved staff: Florian Metzelder, Prof. Dr. Torsten C. Schmidt

Involved students: Matin Funck

Partners: Dr. Thorsten Hüffer, University of Vienna

Funding: German Research Foundation (DFG), Bruno-Werdelmann-Stiftung



The experimental study of weakly sorbing compounds to materials such as multi-walled carbon nanotubes (MWCNTs) may be challenging due to the limited sorbent to solution ratio. As an alternative, column chromatography was therefore used in this project. Adaptation and modification of a method from literature originally developed for soil materials allowed the reproducible packing of stable columns.

Heavy water (D₂O) could be identified as only suitable non-retarded tracer after typically used tracers like inorganic anions (e.g. nitrite) showed significant sorption depending on applied eluent conditions. Especially sorption of inorganic anions was not expected to be that strong. For this reason, the RID approved in this project was necessary for the study.

The influence of a broad range of environmental conditions (pH, ionic strength, and temperature) was successfully studied on sorption of inorganic compounds (initially expected to be useful non-retarded tracers) and organic compounds to MWCNTs. Heterocyclic organic compounds like pyrazole were hardly studied in literature and weak sorption was expected from prediction models. It could be shown that environmental conditions can strongly influence sorption. The advantages of column chromatography like reduced sorbent demand, higher sorbent to solution ratios, high variability in test conditions, and automation potential could be successfully used and pronounce column chromatography as valuable complementary technique in sorption studies.

Furthermore, other sorbent materials than MWCNTs like functionalized MWCNTs, graphene, graphite, and activated carbon could also be studied and compared regarding their sorption properties using the developed column chromatography method allowing the comparison of sorbent materials and effects of for example the surface modification of MWCNTs comparable to batch experiments with strongly reduced sorbent demand.

Consequently, this project demonstrates that column chromatography is suitable as complementary technique in sorption studies for carbon-based materials and nanomaterials to study sorption of weakly sorbing compounds and the influence of environmental conditions on their sorption as well as the comparison of different sorbent materials. In future, column chromatography and its benefits could potentially be used for example in studies using plastic materials as sorbent material investigating the influence of these materials on sorption processes in soils and the aqueous environment. Additionally, column chromatography can be used to derive prediction models for varying environmental conditions for diverse carbon-based materials with reduced time and sorbent demand than necessary for batch experiments.

Marie Skłodowska-Curie Actions Innovative Training Network (MSCA-ITN) “Improved decision-making in contaminated land site investigation and risk assessment” (REMEDIATE)

Involved staff: Nenad Stojanovic (ESR), Dr. Maik A. Jochmann, Prof. Dr. Torsten C. Schmidt

Involved students: Felix Niemann

Partners: Dr. Rory Doherty (Queen’s University Belfast), Dr. Brian Kelleher (Dublin City University), Dr. Frederic Coulon (Cranfield University), Prof. Dr.-Ing. Tim Ricken (TU Dortmund), Dr. Kristian Brandt (University of Copenhagen), Dr. Domenico De Luca (University of Turin),

Funding: EU Commission



The REMEDIATE ITN running until end of 2018 has focused on innovative research and training for the contaminated land site investigation and risk assessment industry in Europe. The REMEDIATE ITN comprised 11 Partners from 6 Member States. REMEDIATE has worked on overarching and advanced approaches to management of contaminated sites. It has addressed site investigations, risk assessment, life cycle assessment and the effectiveness of site remediation. The ultimate goal was to provide a superior level of training for the contaminated land sector, to generate improved decision-making skills for more effective and sustainable remediation. The problem of land contamination across an expanding EU is still highly significant. As a result over €2,000 million is currently spent annually on site risk management. As the EU further develops a common framework for the management of contamination sites, the burden on sustainability, characterisation, risk management and remediation is expanding. REMEDIATE did not address specific remediation technologies but instead the overarching multidisciplinary demands needed for enhanced leadership and decision-making in the future.

At IAC, the project looks specifically into the use of advanced stable isotope methods for site assessments in order to better characterize biodegradation processes of organic contaminants. Being that one of the commonly applied techniques for monitoring the contamination at real sites and investigating their environmental fate is compound-specific stable isotope analysis (CSIA), within the scope of this project we have identified the points of its weaknesses and tried to address them. First one that we have addressed was the need for quick and robust microextraction technique in order to combine extraction, cleanup and sample introduction within one step, while enhancing the sensitivity of the techniques. Following already successfully published solid phase microextraction (SPME) methods, in our work we have improved upon them by careful implementation of recently developed PAL SPME Arrow fibers, that give higher extraction capacity and improved rigidity due to their robust built. The other point of weakness of CSIA that we have addressed was the technical complexity associated with switching between two of the most commonly analyzed elements, carbon and hydrogen. For these purposes we have developed fast and simple switching mechanism that allows dual-element isotope analysis to be done with sample throughput higher than usually.

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

Involved students: Irene M. Sanchez Villalobos

Funding: German Research Foundation (DFG)



Figure 1 Experimental set-up to investigate the mineralization products of nitrogen containing compounds by sulfate-radicals.

The compound-specific isotope analysis (CSIA) of carbon by LC-IRMS is a widely applied method that is used to investigate food authenticity or to get insights into transformation and degradation processes. So far the wet chemical oxidation based technique is restricted to the measurement of carbon isotope ratios. To this end, it is the goal of this project to expand the method for the measurement of nitrogen isotope ratios.

During the course of the project, fundamental changes of the proposed working schedule were necessary. These 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 the wet chemical oxidation by sulfate-radicals. For an in-depth investigation and complete characterization of the mineralization products of nitrogen containing compounds, 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. Especially, the presence of peroxydisulfate was problematic and systematically affected the ammonia fraction of the TN_b determination, in a way that a correction for these measurements had to be developed.

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 heteroaromatically bound nitrogen. These compounds

were far more difficult to oxidize. Here, the degree of oxidation decreases, with increasing number of aromatically bound nitrogen atoms. For such compounds ammonium and nitrate in the same proportion remain as main mineralization products. Additionally, it turned out that the mass balance was by far not complete. (see Figure 2) The acidic oxidation leads into a dead end and is not applicable for LC-IRMS of nitrogen.

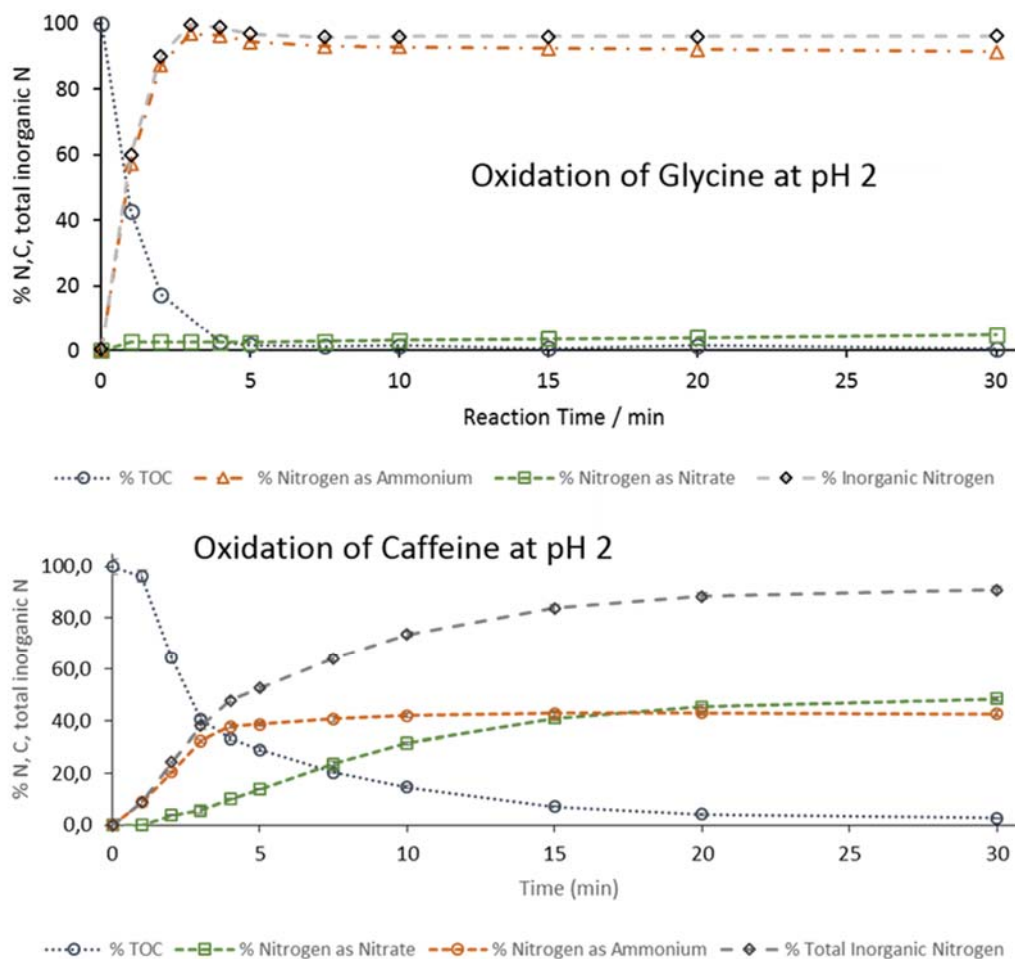


Figure 2 Mineralization of Glycine and Caffeine by sulfate radicals.

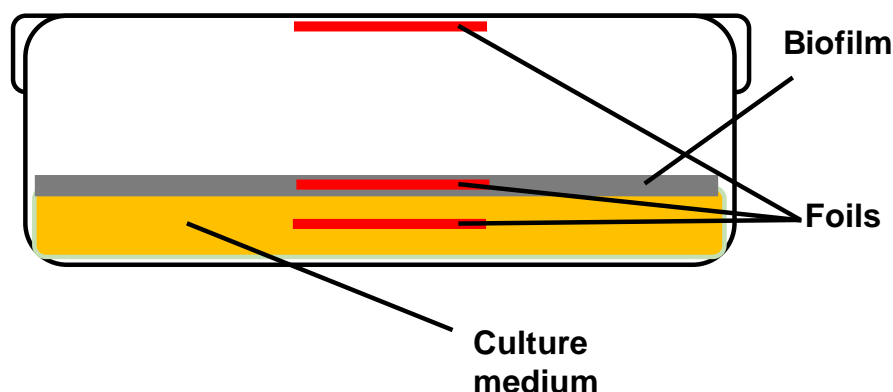
A way out of this dead end was found in the wet chemical combustion under alkaline conditions. The investigation of this process showed mineralization yields of higher 95% for all nitrogen containing compounds with nitrate as only product.

Characterization of the metabolome of *P. aeruginosa* in biofilms as a lung infection model

Involved staff: Timo Köhler (AAC), PD Dr. Ursula Telgheder

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)



P. aeruginosa is an opportunistic pathogenic germ, which leads to nosocomial infection. Especially the lung of cystic fibrosis patients is mostly colonized by this bacterium, in form of a biofilm, and leads to fatal lung infections, which causes the early death of cystic fibrosis patients due to respiratory failures. To increase the life time of cystic fibrosis patients a non-invasive early detection technique is necessary, but still not developed. In this project, the metabolome of *P. aeruginosa* will be characterized considering lung adapted conditions by using a biofilm as a lung infection model. Therefore, a sampling system for the cultivation of *P. aeruginosa* is developed, which enables the sampling of the culture medium, the biofilm and the headspace over time. The sampling of the emitted metabolites, as well as substrates will be done using the thin film microextraction technique (TFME) with PDMS films. This three-phase approach allows the classification of detected and characterized substances as substrates or metabolites.

In the first part of the project, a suitable film material and manufacturer was selected, using TG, TG-MS and TD-GC-MS. Thereafter, the cleaning process for the selected film was optimized with the aim of minimal initial contamination. A suitable separation and detection technique for the loaded films, using a thermo desorption system coupled with a GC-MS was developed. The development of the TD-GC-MS method was carried out using an aqueous solution consisting of twelve standards. The standards were potential metabolites of *P. aeruginosa* and are already published in scientific journals. With the developed method, we are able to identify and quantify several of these possible metabolites down to nanomolar concentrations in a matrix of the nutrient. Furthermore, first TFME experiments using liquid cultures of three different strains of *P. aeruginosa* shows that several metabolites, produced by *P. aeruginosa* can be detected with the developed method. Now we are optimising the developed method with the aim of lower LODs for the potential metabolites and higher peak capacity.

Aromatic amines as biomarkers in human urine using GCxGC: analytical method development and epidemiological studies

Involved staff: Nerea Lorenzo Parodi, Prof. Dr. Torsten C. Schmidt

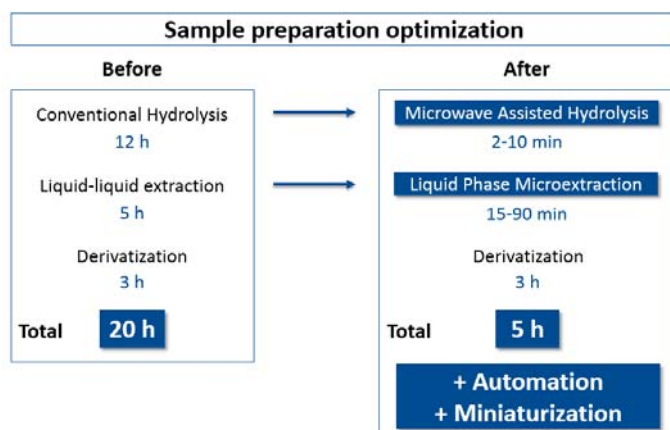
Involved students: Hyerin Kim

Partners: Prof. Dr. Erich Leitner (TU Graz), Dr. Astrid Gjelstad (Univ. of Oslo), Prof. Dr. Susanne Moebus (Uniklinikum Essen)

Funding: Evonik Industries AG

Several aromatic amines pose a health threat due to their carcinogenic effects. One of the most important exposure routes to these compounds is through tobacco smoke. After being inhaled, the aromatic amines enter the bloodstream and can be transported to the liver, where they are metabolized, and eventually reach the bladder. Once in the bladder, the metabolites can either be excreted with the urine or form DNA and protein adducts that can induce bladder cancer.

Sample preparation procedures for the analysis of aromatic amines with GC-MS usually involve time consuming and labor intensive steps. The first part of the project aims to minimize this burden by substituting the conventional approach with a more efficient one. The individual steps are compared with alternative ones (conventional vs. microwave assisted hydrolysis and liquid-liquid extraction (LLE) vs. liquid phase microextraction) and the best performing option is chosen for future experiments.



First aim: automation, miniaturization and increased efficiency of the sample preparation steps.

Microwave assisted hydrolysis was tested and compared to conventional hydrolysis. Conventional hydrolysis was proven to be better for the samples at hand and easier to operate. Furthermore, three phase HF-LPME and PALME were studied and compared to the conventional liquid-liquid extraction step. PALME showed promising results, however, due to the limited amount of sample used, not enough sensitivity was achieved.

Thanks to the collaboration with Prof. Dr. Susanne Moebus, involved in the projects Heinz Nixdorf Recall study (over 4.800 participants) and Heinz Nixdorf MehrGenerationenStudie (3 generations), we have access to urine samples and medical information from the participants. In order to achieve a high throughput and have access to the limited archived samples, automation and miniaturization of the sample preparation procedure are also key components of the sample preparation optimization. Therefore, the conventional LLE step will be automated, and smaller sample volumes and more sensitive techniques, such as NCI-GC-MS or GC-MS/MS, will be tested.

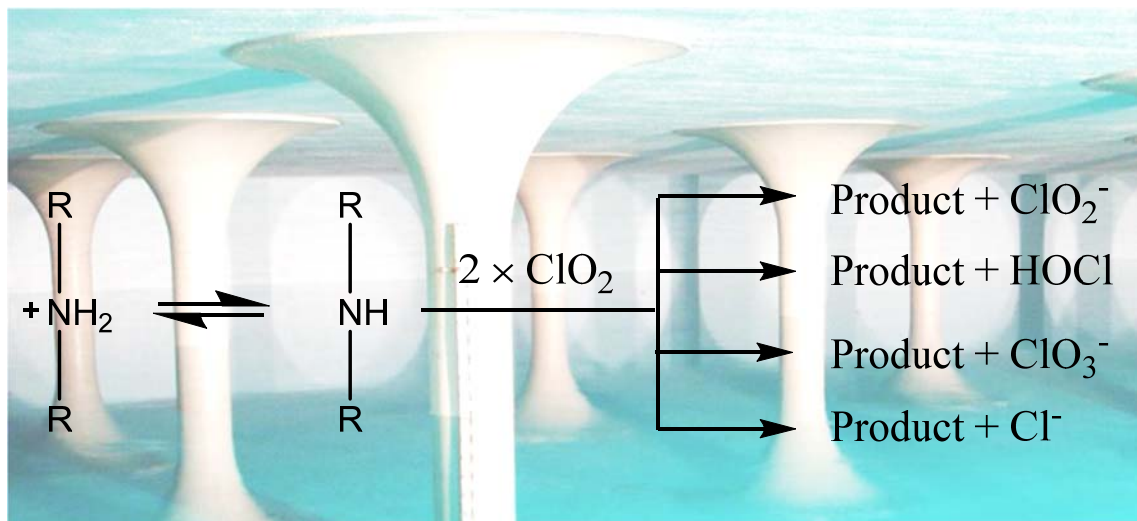
Finally, once the optimized method is established, a statistically relevant number of samples will be measured. Afterwards, the correlations between the aromatic amines present in the samples (amounts and types), the smoking status of the donor (smoker, non-smoker and passive smoker) and the development of smoking related diseases will be studied using complex statistical methods.

Reactions of chlorine dioxide with nitrogen-containing compounds

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

Involved students: Xenia Mutke, Katharina Hupperich

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 treatment of water since several decades. However reaction mechanisms of pollutant degradation are hardly known. With support of a DAAD scholarship, reactions of nitrogen-containing compounds with chlorine dioxide are investigated. Organic pollutants, though, are very complex and often reveal several reactive sites which can react with chlorine dioxide, what aggravates their investigation. Hence, the present project focuses on simple model compounds which reveal only one site of reaction towards chlorine dioxide such as saturated *N*-heterocycles (e.g., piperidine).

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 ClO₂ 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 can be formed as the product of the second reaction. The results have shown that for piperazine, a second electron transfer reaction with the second nitrogen forms another chlorite and a transformation product which after an imine formation and further hydrolysis will form formaldehyde and ethylenediamine. This was confirmed with more than 80% formation of chlorite as the major ClO₂ transformation product. But in case of 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.

To further verify the knowledge gained by these compounds, reaction of cetirizine (antihistamine) with ClO₂ was investigated and it was observed that the second attack in case of this tertiary amine forms chlorite as well. Formation of chloride and chlorate was also observed, although not as pronounced as chlorite and HOCl.

Theses completed in 2018

PhD Theses



31.01.2018

Alyson Rogerion Ribeiro

“Fate and effects of two veterinarian cephalosporins, ceftiofur and cefapirin, in the aquatic environment”

Summary

Human and veterinary cephalosporins can reach the environment due to their widespread consumption, intermittent and diffuse discharge rate. Particular attention is given to this antibiotic group due to their broad spectrum of activity and possible deleterious effects in non-target organisms as well as pressure in antimicrobial resistance acquisition, which may be caused by the parental drugs, metabolites and bioactive byproducts.

Physicochemical properties, consumption, occurrence in aqueous matrices, available ecotoxicity data and technical strategies employed for the degradation of compounds within this group were critically discussed. Classical biological treatment systems cannot provide complete removal of cephalosporins, therefore several technologies have been employed for the removal of these compounds from aquatic matrices. In this regard, photolysis and mass transfer processes were the most investigated ones. Cefalexin, cefradine, cefotaxime and cefazolin possess respectively the highest occurrence score in the aquatic environment. Topics were identified where further investigations are necessary, as: ecotoxicological assessment of parental and transformed compounds, especially using soil organisms, cyanobacteria and biofilms; abiotic degradation rates (hydrolysis, photolysis) and control of natural degradation during abatement technologies; analysis of biologic inactivation and inclusion of metabolites and transformation products in surface water surveillance.

Several biotic and abiotic processes in the environment depend primarily on the xenobiotic pH-dependent speciation. The veterinarian drugs ceftiofur (CEF) and cefapirin (CEPA) are widely used for the treatment of recurrent and economically relevant infections. The acid dissociation constants (pKa) of CEF and CEPA were studied using two experimental techniques (potentiometry and spectrophotometry) along with computational simulations. In silico studies were also used to contrast and discuss the experimental dissociation constants available in the literature of 14 cephalosporins. pKa values were obtained experimentally for CEF (2.68 ± 0.05 , carboxylic acid group deprotonation) and for CEPA (2.74 ± 0.01 for the carboxylic acid deprotonation and 5.13 ± 0.01 for the pyridinium ring deprotonation). The pKa values available for cephalosporins (n=88) agreed with the in silico predicted data (ACD/Percepta RMSE: 0.552 and Marvin RMSE: 0.706). Therefore, in the biologically and environmentally relevant pH values of 6 - 7.5, CEF and CEPA, as well as many other cephalosporins, are present as anionic species.

CEF and CEPA have been detected in aquatic environments and their fate in surface water as well as during drinking water processing is still unknown. To understand the persistence of cephalosporins in aqueous matrices, hydrolytic and photolytic kinetics were investigated. Both CEF and CEPA showed high instability under alkaline conditions, degrading in few minutes at $\text{pH} > 11$ ($T = 22 \pm 1^\circ\text{C}$). Cephalosporins speciation did not significantly influence the direct photolysis rates of CEF and CEPA under simulated water disinfection radiation (UV-C, $\lambda = 254 \text{ nm}$). All ionic species of CEF ($k_{\text{app}} 0.0095 \pm 0.0004 \text{ MJ cm}^{-2}$) and CEPA ($k_{\text{app}} 0.0092 \pm 0.001 \text{ MJ cm}^{-2}$) presented fast and similar pseudo-first order degradation rates. In hydrolysis experiments using surface water CEF showed a significant matrix-dependent stability increase with a half-life ($t_{1/2}$ 14.7 d) tenfold higher than in buffered solutions ($t_{1/2}$ 1.4 d). Meanwhile, CEPA showed similar hydrolysis in buffered solutions ($t_{1/2}$ 3 d) and in river water ($t_{1/2}$ 4.2 d). On the other hand, this antibiotic showed subtle faster photo-degradation rate in this same matrix ($k_{\text{app}} 0.0128 \pm 0.001 \text{ MJ cm}^{-2}$), while CEF photo-degradation showed no matrix effects.

The acute and chronic toxicities of CEF and CEPA towards aquatic organisms were also investigated. CEF and CEPA have significant decay during cladocera (*Daphnia magna*) tests, portraying half-life times ($t_{1/2}$) of 49 and 53 hours, respectively. During tests with green algae (*Scenedesmus spec.*), CEPA was more instable ($t_{1/2}$ 88 h) than CEF ($t_{1/2}$ 267 h). CEF and its hydrolysis products induced deleterious effects in *Daphnia magna* (48h EC₅₀ 139, LC₅₀ 179 in μM), which was not observed with *Scenedesmus spec.* (72h NOAEC $82.5 \pm 2.5 \mu\text{M}$). In the case of CEPA, no toxic effects were observed in both tests (48h EC-LC₅₀ > 510 and 72h NOAEC 57 ± 6 , in μM). The effects of water disinfection radiation (UV-C, $\lambda = 254 \text{ nm}$) on ecotoxicological responses were also studied. Photolysis of CEPA resulted in toxic products, which were effective for cladocera but not for the green algae. On the other hand, the different radiation doses studied did not affect CEF ecotoxicity. This work should provide important data for researchers interested in cephalosporins antibiotics as environmental contaminants, confirming the importance of investigating the fate and effects of cephalosporin antibiotics in the aquatic environment.



08.02.2018

Frank Hitzgrath

“Determination of diffusible hydrogen in high-strength steels with respect to the lattice structure”

Summary

In order to meet the increasing material requirements of the automotive industry, the development of novel, high-strength steels enforced in the steel industry. One of the problems to be solved is the hydrogen-induced cracking, which can occur even at low hydrogen contents in the steel. Particular attention should be paid to the diffusible hydrogen. One often used analysis method is the TD-MS method. This method is used to determine diffusible and trapped hydrogen and to determine the desorption energy of hydrogen in high-strength steels. The aim of this work was to establish a correlation between the desorption energy of diffusible and "trapped" hydrogen with the structure of the steel. In order to be able to establish the correlation between the desorption energy of the hydrogen and the structure of the steel, the TD-MS analysis method had to be optimized. The optimizations were necessary to investigate influences on the analytical procedure, which could falsify the analytical results. For optimization, possible possibilities of influencing the method were investigated. Experiments in which the influence of the carrier gas on the analysis method were examined, showed that the alloying elements manganese, titanium and an alloyed steel sample, a hydrogen signal at about 450 ° C is detected, which does not originate from the analytical sample. This signal comes from the catalytic water decomposition of the residual moisture in the carrier gas. This effect is due to the different oxygen affinities of the elements. For the determination of the desorption energy, it was necessary to develop a method with which the sample temperature can be measured accurately. Due to the fact, that the temperature measurement of TD-MS is too inaccurate, an external temperature measurement method has been developed. With a thermocouple, in which the tip was bent into a loop, the most reproducible results were achieved. The sample is clamped in the loop and has permanent firm contact with the probe.

Loading experiments have shown that the amount of hydrogen absorbed depends on various factors. These include, for example, the sample thickness, the loading method, the surface condition of the sample and the sample composition. In addition to the optimization measures, the influence of the microstructure on the trapped hydrogen content was investigated

When determining desorption rates of diffusible hydrogen in operational samples, it was found that the materials containing carbide precipitates do not always contain trapped hydrogen. Further experiments indicated that trapped hydrogen was only found in the processed materials. In experiments with the same material in the laboratory, no trapped hydrogen could be detected. Probably the reason for this lies in the production steps in which the material is rolled and processed.

This material processing changes the microstructure so that diffusive hydrogen attaches to lattice defects.

For the further investigation of trapped hydrogen, samples with different microstructures were produced. Among other things, a pure martensitic structure was created. For this different temperature programs were used. Trapped hydrogen would have been expected in the prepared lattice structures, but none could be detected. This is probably also because the material was not processed (rolled, drawn, etc.). The deformation seems to influence the property of hydrogen storage in the material.

Reproducible the trapped hydrogen was analyzed in deformed samples with pearlitic structure. It has been found that the material must be deformed so that trapped hydrogen can be detected during the measurement. The results of the tensile tests with this material suggest that the degree of deformation is responsible for whether trapped hydrogen is present. This is confirmed by thermoforming tests according to DIN 8584.



20.04.2018

Alexandra Fischbacher

“Formation and Quantification of $\cdot\text{OH}$ in oxidative water treatment”

Summary

$\cdot\text{OH}$ are unselective and fast reacting. Water treatment processes leading to $\cdot\text{OH}$ are called advanced oxidation processes (AOPs). The Fenton process, one of several AOPs, describes the reaction of Fe(II) with hydrogen peroxide. Fe(II) is oxidized to Fe(III) that reacts with hydrogen peroxide to Fe(II) and again initiates the Fenton reaction. One reactive species formed in the Fenton process are $\cdot\text{OH}$. Conditions such as pH, the $\text{H}_2\text{O}_2:\text{Fe}(\text{II})$ ratio and ligand concentration may influence the $\cdot\text{OH}$ yield. It could be shown that at $\text{pH} < 2.7$ and > 3.5 the $\cdot\text{OH}$ yield decreases significantly. The investigated ligands were pyrophosphate and sulfate. It was found that pyrophosphate forms a complex with Fe(III) that does not react with hydrogen peroxide and thus, terminates the Fenton process and decreases the $\cdot\text{OH}$ yield. Sulfate also influences the Fenton process but not to the same extent as pyrophosphate. The $\cdot\text{OH}$ yield is decreased when sulfate is added but even at higher concentrations the Fenton reaction is not terminated. It is necessary to investigate more conditions inhibiting or enhancing the Fenton process to be able to predict and control the reaction.

Another AOP that was dealt with is the peroxone process. It describes the reaction of O_3 with H_2O_2 . Hitherto, it has been assumed that the $\cdot\text{OH}$ yield is unity with respect to O_3 consumption. Three approaches were conducted to investigate the $\cdot\text{OH}$ per consumed O_3 . The first approach included

competition experiments. The consumption of trace compounds (4-chlorobenzoic acid, 4-nitrobenzoic acid and atrazine present in trace amounts) has been followed as a function of the O_3 concentration in a solution containing H_2O_2 and tertiary butanol (tBuOH) in high excess over the trace compounds. For comparison the experiments were conducted with authentic $\cdot OH$ generated by γ -radiolysis. By means of known $\cdot OH$ rate constants the competition was adequately fitted. Fitting the peroxone data, however, the consumption of the trace indicators can only be rationalized if the $\cdot OH$ yield is near 0.5 (4-chlorobenzoic: 0.51; 4-nitrobenzoic: 0.45; atrazine: 0.6). Beside the competition experiments further evidence for a reduced $\cdot OH$ yield (near 0.5) is derived from a product analysis of the reactions of tBuOH with $\cdot OH$ and dimethyl sulfoxide with $\cdot OH$. The mechanistic interpretation for the low $\cdot OH$ yield is as follows. In the reaction of O_3 with HO_2^- an adduct (HO_5^-) is formed that decomposes into $O_3^{\cdot -}$ and HO_2^{\cdot} in competition with $2 O_2 + OH^-$. The latter process contributes to a reduced $\cdot OH$ yield. From the mechanistic considerations and the experimental data it is concluded that the $\cdot OH$ yield per consumed O_3 must be near 0.5. As $\cdot OH$ are also formed from the reaction of O_3 with water matrix components the effect of the revised mechanisms on practical implementations cannot be predicted.

Ozone is often used in drinking water treatment. In dependency on the water matrix constituents different undesired by-products may be formed. If the water to be treated contains bromide ozonation of this water leads to bromate formation, as the reaction of bromide with ozone yields bromate. Bromate is regulated in drinking water as it is considered to be carcinogenic. Its formation is a multistep process resulting in the last step from the reaction of ozone with bromite. Although this process seemed to be established, it has been shown that ozone reacts with bromite not as previously assumed via O-transfer but via electron-transfer. Besides bromate, the electron transfer reaction also yields $O_3^{\cdot -}$, the precursor of $\cdot OH$. In the experimental setup $\cdot OH$ were not produced from O_3 self-decomposition but solely by the electron-transfer reaction. The first evidence for the electron transfer reaction is derived from the addition of tBuOH as $\cdot OH$ scavenger and measuring formaldehyde, the product from the reaction of tBuOH with $\cdot OH$. To confirm the outcome of the first experiments HOBr (formed from the reaction of O_3 and bromide) and bromate yields were measured in systems with and without tBuOH. As $\cdot OH$ contribute to bromate formation, higher bromate and HOBr yields were observed in the absence of tBuOH than in its presence, where all $\cdot OH$ are scavenged. Based on the presented results, a pathway from bromide to bromate, revised in the last step, was suggested. The revised reaction step may help in modelling bromate formation as it is hitherto very imprecise due to too many included reactions that are not well known.

The quantification of $\cdot OH$ is of great interest and its exact quantification is essential for mechanistic considerations. An established method for the determination of $\cdot OH$ in water is the product analysis of the products from the reaction of tBuOH with $\cdot OH$, that is also used in this thesis. The products of this reaction are beside formaldehyde and acetone 2-methyl-2-hydroxypropanol and 2-methyl-2-hydroxypropanal. The latter two are not commercially available and therefore, an indirect quantification of $\cdot OH$ is just possible by an assumed yield of formaldehyde formed per $\cdot OH$. The synthesis of 2-methyl-2-hydroxypropanol was performed by adapting a previously published synthesis. The product of the synthesis was characterized by NMR and GC-MS and 2-methyl-2-hydroxypropanol was identified. One method to synthesize 2-methyl-2-hydroxypropanal is the oxidation of 2-methyl-2-hydroxypropanol by Dess-Martin periodinane (DMP). The product characterization was done by NMR and HPLC-UV after derivatization. The NMR spectra did not show any product and the HPLC chromatogram shows many impurities and therefore, 2-methyl-2-hydroxypropanal could not be identified. To obtain the desired product further oxidation methods have to be applied and as 2-methyl-2-hydroxypropanol is just formed from one reaction in the cascade of reactions its importance for the quantification of $\cdot OH$ is still unknown..



09.08.2018

Florian Metzelder

“Investigation of sorption properties of carbon nanomaterials using packed columns and inverse liquid chromatography”

Summary

Sorption studies on carbon-based materials and carbon-based nanomaterials (CNMs) like multiwalled carbon nanotubes (MWCNTs) are typically conducted using batch experiments. This experimental approach is simple to perform and gives reliable results for most sorbates. However, weakly sorbing compounds may be challenging due to a limited sorbent to solution ratio. Here, column chromatography using sorbent packed columns for the determination of sorption data like distribution coefficients (K_d) can be a promising complementary approach offering significantly higher sorbent to solution ratios enabling the analysis of weakly sorbing compounds. This approach was already used for sorption studies on soils. Mandatory for this experimental approach is a non-retarded tracer, showing no interaction with the sorbent material as this is necessary as reference point for the calculation of K_d values. Furthermore, reversible sorption using pulse injection of the investigated sorbates is mandatory as otherwise no sorption data could be calculated. To this end, this thesis aims at the investigation of the suitability of column chromatography for sorption studies on CNMs and especially MWCNTs for weakly sorbing compounds.

Adaptation and modification of a method from literature originally developed for soil materials allowed the reproducible packing of stable columns. Main characteristics of packed columns like porosity and bulk density varied by less than 3 % relative standard deviation. Heavy water (D_2O) could be identified as only suitable non-retarded tracer after typically used tracers like inorganic anions (e.g. nitrite) showed significant sorption depending on applied eluent conditions regarding ionic strength. The influence of a broad range of environmental conditions (pH, ionic strength, and temperature) was successfully studied on sorption of inorganic compounds (initially expected to be useful non-retarded tracers) and organic compounds to MWCNTs. Heterocyclic organic compounds like pyrazole were hardly studied in literature and weak sorption was expected from prediction models. It could be shown that environmental conditions can strongly influence sorption. Sorption reduced with increasing temperature indicating an exothermic process and the contribution of H-bonding to overall sorption. Ionic strength strongly affected sorption of inorganic anions while the effect on organic sorbates was lower. Sorption of for example iodide was reduced by 90 % or completely suppressed for bromide and nitrite when increasing NaCl concentration from 1 to 100 mM. A key factor in sorption of inorganic and organic sorbates was the pH value as it was previously shown in literature for selected compounds using batch experiments. Electrostatic attraction of negatively charged inorganic anions to the oppositely charged sorbent surface at pH 3 increased sorption about factor ten compared to electrostatic repulsion conditions at pH 9. For ionizable organic compounds of this study (e.g. pyridine or imidazole) electrostatic repulsion was observed at pH 3 due to the similar positive charges of sorbent and sorbate reducing sorption by 80 % compared to pH 9 where the sorbates were not charged. Therefore, electrostatic interactions can increase or reduce, but not prevent sorption. Other sorbent materials than MWCNTs like functionalized MWCNTs, graphene, graphite, and activated

carbon could also be studied and compared regarding their sorption properties using the developed column chromatography method allowing the comparison of sorbent materials and effects of for example the surface modification of MWCNTs comparable to batch experiments with strongly reduced sorbent demand.

Consequently, this thesis demonstrates that column chromatography is suitable as complementary technique in sorption studies for carbon-based materials and nanomaterials to study sorption of weakly sorbing compounds and the influence of environmental conditions on their sorption as well as the comparison of different sorbent materials. Relationships and trends regarding the influence of environmental conditions or material modifications observed using batch experiments could also be confirmed using column chromatography and extended to other sorbates. Using column chromatography, time and sorbent material demand for isotherm determination could be reduced and the automation potential increased showing the benefits of this methodology compared to batch experiments. In future, column chromatography and its benefits can be used for example in studies using plastic materials as sorbent material investigating the influence of these materials on sorption in soils and the aqueous environment.



31.10.2018

Oliver Knoop

“Formation and Effects of Transformation Products during the Ozonation of Tamoxifen”

Summary

To reduce the amount of micropollutants and their ecotoxicological effects released into the environment via wastewater treatment plant (WWTP) effluents, ozonation showed to be suitable and is broadly discussed as advanced wastewater treatment (AWT) in combination with subsequent biological filtration. Especially endocrine effects can be induced at low concentrations of a broad range of micropollutants. Estrogenic and androgenic effects are diminished due to ozonation and the reactions of compounds inducing these effects are well investigated. In contrast, the corresponding antagonistic effects have recently been reported to be resilient to this treatment strategy and until now, only little information for the reaction of anti-estrogenic compounds with ozone is available. For this reason, this study focuses on the reaction of tamoxifen (TAM), a selective estrogen receptor modulators (SERM), with ozone, the formation of transformation products (TPs), and the simultaneous progression of anti-estrogenic activity and acute ecotoxicological effects.

All experiments were performed in ultra-pure water in presence of radical scavengers to rule out radical reactions and focus solely on the reaction of TAM and ozone, including the dissociation of TAM in dependency of the pH. Reaction kinetics were investigated using a competition kinetics approach over a broad range of pH to determine the second order rate constants for the reactions of ozone with the corresponding species of TAM. Rate constants differed substantially between the two relevant

TAM species ($k(\text{TAM}, \text{O}_3) = 3.25 \times 10^8 \text{ M}^{-1} \text{ s}^{-1}$; $k(\text{TAM-H}^+, \text{O}_3) = 1.57 \times 10^4 \text{ M}^{-1} \text{ s}^{-1}$), resulting in an apparent second order rate constant of $> 10^6 \text{ M}^{-1} \text{ s}^{-1}$ at pH 7. Hence, full abatement by ozonation as AWT can be assumed. However, for the neutral species with a tertiary amine as most reactive moiety towards ozone, the species specific second order rate constant obtained is unexpectedly high.

Five TPs were identified in total using high resolution mass spectrometry and structure elucidation based on fragmentation in tandem mass spectrometry. Two primary TPs, TP 270 (Criegee product) and TP 388 (hydroxylation), are formed during the ozonation of the corresponding acid of TAM. TAM-N-oxide is the primary product formed in the reaction of the neutral TAM species and ozone and was unequivocally identified using a reference standard. Further oxidation of the primary TPs by ozone results in the formation of the two secondary TPs TP 286 and TP 404, the corresponding N-oxides of TP 270 and TP 388.

Anti-estrogenic activity using the *Arxula adenivorans* yeast estrogen screen (A-YES) assay, and acute toxicity for *Daphnia magna* and growth inhibition of the green algae *Desmodesmus subspicatus* were monitored in dependence of the ozone dose, to allow correlation analysis with the formation of TPs. The anti-estrogenic activity was proliferated with increasing ozone dose, even after full abatement of TAM, and the residual effect correlated to the formation of TP 270. The formation of N-oxides was on the other hand coherent with a loss of the anti-estrogenic activity. The observed immobilization of *D. magna* was removed at low ozone doses completely. An increase of the algae growth inhibition with an increasing ozone dose was observed, which correlated again with the formation of TP 270, as well as TP 388. At pH 3, ozonation of TAM resulted in a duplication of both effects, anti-estrogenic activity and algae growth inhibition. The main observed TP here was TP 270, which was identified as 4-(Dimethylaminoethoxy)-benzophenone. Due to the high risk potential of TP 270, a new purification strategy was successfully developed for obtaining pure TP270 for further toxicity testing by synthesis. This study elucidated the reaction of the SERM TAM with ozone and the formation of primary and secondary TPs. Additionally, the formation of toxicologically relevant TPs was demonstrated. Therefore, this study might help to understand the persistence of anti-estrogenic effects in ozonation as AVT. To further foster our understanding in that regard, future studies need to further investigate the ozonation of SERMs, including metabolites, formation of TPs in wastewater, and their removal in subsequent biological filtration.



28.11.2018

Xolelwa Lamani-Dixon

“Analysis of aromatic amines in human urine using comprehensive multi-dimensional gas chromatography mass spectrometry”

Summary

Over the years, it has been revealed that some aromatic amines (AAs) have a potential to cause bladder cancer in humans, with cigarette smoking as a major source. However, in relation to tobacco-smoking bladder cancer only few of these compounds have been reported. Hence, an interest to study more about the existence of AAs in human body fluids was developed. The use of a comprehensive multi-dimensional gas chromatography mass spectrometry (GC×GC-qMS) enabled the detection of several isomeric compounds of the same molecular mass and it has given a clear picture of the existence of aromatic amines in human urine due to its fingerprint analysis. For the investigation of urine samples, which were of smokers, non-smokers and past-smokers in this study; pre-treatment steps are necessary prior to analysis to make the analytes suitable for GC. The steps include: (i) thermal acidic hydrolysis to cleave aromatic amine adducts, (ii) liquid-liquid extraction (LLE) of the hydrolyzed analytes, (iii) derivatization of the extracted amines through diazotization and iodination and (iv) enrichment of the iodinated derivatives with headspace solid-phase microextraction (SPME), before introducing the analytes into the GC system. The application of the developed in-situ derivatization SPME GC×GC-qMS technique resulted in more than 100 isomeric aromatic amines identified in human urine and with regard to the numbers and peak intensities, the urine of smokers were more burdened compared to non- and past-smokers urine. Also, some alternative developments were investigated in order to improve sample preparation procedures which are mainly the time and solvents consumed during preparation. Microwave-assisted technique showed a possibility of potentially minimizing the time from 12 hours of the conventional hydrolysis to ≤ 1 hour. And for the organic solvents, less amounts were achieved by thin-film microextraction (TFME) including the amount of sample needed. In conclusion, the work done here offers a better understanding on the prevalence of several aromatic amines in humans, than previously reported. This creates a platform for further investigations probably in the urine samples of the patients who are diagnosed with bladder cancer. This may eventually be useful in finding biomarkers which could be used to determine the level of cancer-causing aromatic amines in urine samples.

Master Theses

Katharina Hupperich

„Formation of secondary oxidants and by-products in chlorine dioxide based treatment of water“

Ibrahim Malash

„Comparision of three consumer test methods to investigate consumer inspired chemical quality“

Astrid Mayer

„Target and non-target screening of organic micropollutants in the river Rhine and its main tributaries using GC-DBDI-HRMS“

(at eawag, Host supervisor: Heinz Singer)

Yanina Müller

„Identification and Quantification of Microplastics in the Longitudinal Profile of the River Elbe, Germany“

(at TZW Karlsruhe, Host supervisors: Dr. Florian Storck, Dr. Nicole Zumbülte)

Dennis Münchrath

„Abbau von Nitrat/Nitrit in Wässern durch leuchtstoffhaltige Xenon-Excimerstrahler“

(at DLR, Host supervisor: Dr. Christian Jung)

Xenia Mutke

„Investigation of reactions of saturated heterocyclic amines with chlorine dioxide“

Irene María Sánchez Villalobos

„Study of phosphorus recovery from sewage sludge for the development of sustainable value chains on the basis of the framework conditions in the Emscher-Lippe-Region“

Bachelor Theses

Christoph Bugdoll

„Entwicklung eines Betreiber freundlichen Messverfahrens zur Quantifizierung des Säurespektrums bei kombinierter Wasserstoff- und Methangas Produktion“

Robert Marks

„Untersuchungen zum Abbau von organischen Verbindungen unter Verwendung von gepulsten bordotierten Diamantelektroden“

Anna-Lena Röhrig

„Qualitativer und quantitativer Nachweis von Aktivkohle in Kläranlagenabläufen und Belebtschlamm“

Kristina Speer

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

Samuel Thebingbuß

„Reaktion von stickstoffhaltigen Verbindungen mit Ozon“

Lucie Tintrop

„Grundlegende Untersuchungen zu der Ozonung von verschiedenen Phenolderivaten“

Publications

Peer-reviewed Journals

1. O. Knoop, L. L. Hohrenk, H. V. Lutze, T. C. Schmidt:
Ozonation of Tamoxifen and Toremfene – Reaction Kinetics and Transformation Products
Environ. Sci. Technol. **52** (2018), 12583-12591
DOI: 10.1021/acs.est.8b00996
2. V. Hinnenkamp, J. Klein, S. W. Meckelmann, P. Balsaa, T. C. Schmidt, O. J. Schmitz:
Comparison of CCS Values Determined by Traveling Wave Ion Mobility Mass Spectrometry and Drift Tube Ion Mobility Mass Spectrometry
Anal. Chem. **90** (2018), 12042-12050
DOI: 10.1021/acs.analchem.8b02711
3. M. Schulte, M. A. Jochmann, T. Gehrke, M. Denecke, T. C. Schmidt:
Carbon isotopic fractionation via diffusion in a coarse material
Geochemistry, Geophysics, Geosystems **19** (2018), 3246-3253
DOI: 10.1029/2017GC007378
4. F. Metzelder, M. Funck, T. Hüffer, T. C. Schmidt:
Comparison of sorption to carbon-based materials and nanomaterials using inverse liquid chromatography
Environ. Sci. Technol. **52** (2018) 9731-9740
DOI: 10.1021/acs.est.8b01653
5. J. Terhalle, P. Kaiser, M. Jütte, J. Buss, S. Yasar, R. Marks, H. Uhlmann, T. C. Schmidt, H. V. Lutze:
Chlorine dioxide – Pollutant transformation and formation of hypochlorous acid as secondary oxidant
Environ. Sci. Technol. **52** (2018), 9964-9971
DOI: 10.1021/acs.est.8b01099
6. A. R. Ribeiro, B. Sures, T. C. Schmidt:
Cephalosporin antibiotics in the aquatic environment: A critical review of occurrence, fate, ecotoxicity and removal technologies
Environ. Pollut. **241** (2018), 1153-1166
DOI: 10.1016/j.envpol.2018.06.040
7. O. Knoop, M. Woermann, H. V. Lutze, B. Sures, T. C. Schmidt:
Ecotoxicological effects prior to and after the ozonation of Tamoxifen
J. Hazard. Mat. **358** (2018), 286-293
DOI: 10.1016/j.jhazmat.2018.07.002
8. A. Barion, P. Balsaa, F. Werres, U. Neuhaus, T. C. Schmidt:
Stability of organochlorine pesticides during storage in water containing sediment and on loaded SPE disks
Chemosphere **210** (2018), 57-64
DOI: 10.1016/j.chemosphere.2018.06.173
9. S. Dobaradaran, T. C. Schmidt, I. Nabipour, N. Khajeahmadi, S. Tajbakhsh, R. Saeedi, M. Javad Mohammadi, M. Keshtkar, M. Khorsand, F. Faraji Ghasemi:
Characterization of plastic debris and association of metals with microplastics in coastline sediment along the Persian Gulf
Waste Manag. **78** (2018), 649-658
DOI: 10.1016/j.wasman.2018.06.037

10. T. C. Schmidt:
Recent trends in water analysis triggering future monitoring of organic micropollutants
Anal. Bioanal. Chem. **410** (2018), 3933-3941
DOI: 10.1007/s00216-018-1015-9
11. T. Bohners, M. Kelch, B. Gebert, X. L. Osorio Barajas, T. C. Schmidt, J. S. Gutmann, J. Müssig:
Improvement of fibre-matrix adhesion in cellulose/polyolefin composite materials by means
of photo-chemical fibre surface modification
Cellulose **25** (2018), 2451-2471
DOI: 10.1007/s10570-018-1724-4
12. M. Dronov, T. C. Schmidt, J. Schram:
Concentration-Gradient-Method for sulphur and strontium isotope ratio determination by
quadrupole-based ICP-MS in gypsum
Rapid Comm. Mass Spectrom. **32** (2018), 567–575
DOI: 10.1002/rcm.8067
13. S. Dobaradaran, T. C. Schmidt, I. Nabipour, A. Osotovar, A. Raeisi, R. Saeedi, M. Khorsand, N.
Khajeahmadi, M. Keshtkar:
Cigarette butts abundance and association of mercury and lead along the Persian Gulf beach:
an initial investigation
Environ. Sci. Pollut. Res. **25** (2018), 5465-5473
DOI 10.1007/s11356-017-0676-9
14. D. Koester, J.-B. Wolbert, M. Schulte, M. A. Jochmann, T. C. Schmidt:
The origin of xylitol in chewing gum – a compound-specific isotope technique for the
differentiation of corn and wood based xylitol by LC-IRMS
J. Agric. Food Chem. **66** (2018), 2015-2020
15. S. Willach, H. V Lutz, K. Eckey, K. Löppenberg, M. Lüling, J.-B. Wolbert, D. M. Kujawinski, M.
A. Jochmann, U. Karst, T. C Schmidt:
Direct photolysis of sulfamethoxazole using various irradiation sources and wavelength
ranges - insights from degradation product analysis and compound-specific stable isotope
analysis
Environ. Sci. Technol. **52** (2018), 1225-1233
DOI: 10.1021/acs.est.7b04744
16. A. R. Ribeiro, H. V. Lutz, T. C. Schmidt:
Base-catalyzed hydrolysis and speciation-dependent photolysis of two cephalosporin
antibiotics, Ceftiofur and Cefapirin
Water Res. **134** (2018), 253-260
DOI: 10.1016/j.watres.2017.12.048
17. G. Renner, T. C. Schmidt, J. Schram:
Analytical Methodologies for Monitoring Micro(nano)plastics: Which are Fit for Purpose?
Current Opinion Environ. Sci. Health **1** (2018), 55-61
DOI: 10.1016/j.coesh.2017.11.001
18. F. Metzelder, M. Funck, T. C. Schmidt:
Sorption of heterocyclic organic compounds to multi-walled carbon nanotubes
Environ. Sci. Technol. **52** (2018), 628–637
DOI: 10.1021/acs.est.7b05205
19. F. Itzel, K. S. Jewell, J. Leonhardt, L. Gehrman, U. Nielsen, T. A. Ternes, T. C. Schmidt, J.
Tuerk:
Comprehensive analysis of antagonistic endocrine activity during ozone treatment of hospital
wastewater
Sci. Tot. Environ. **624** (2018), 1443-1454

20. O. Knoop, F. Itzel, J. Tuerk, H. V. Lutze, T. C. Schmidt:
Endocrine effects after ozonation of tamoxifen
Sci. Tot. Environ. **622-623** (2018), 71-78
DOI: 10.1016/j.scitotenv.2017.11.286
21. A. R. Ribeiro, B. Sures, T. C. Schmidt:
Ecotoxicity of the two veterinarian antibiotics ceftiofur and cefapirin before and after photo-transformation
Sci. Tot. Environ. **619-620** (2018), 866-873
DOI: 10.1016/j.scitotenv.2017.11.109
22. H. V. Lutze, J. Brekenfeld, S. Naumov, C. von Sonntag, T. C. Schmidt:
Degradation of perfluorinated compounds by sulfate radicals – New mechanistic aspects and economical considerations
Water Res. **129** (2018), 509-519
DOI: 10.1016/j.watres.2017.10.067
23. E. Reisz, C. von Sonntag, A. Tekle-Röttering, S. Naumov, W. Schmidt, T. C. Schmidt:
Reaction of 2-propanol with ozone in aqueous media
Water Res. **128** (2018), 171-182
DOI: 10.1016/j.watres.2017.10.035
24. M. Dronov, T. Koza, A. Schwiers, T.C. Schmidt, J. Schram:
Strontium carbonate precipitation as a sample preparation technique for isotope ratio analysis of Sr in mineral water and wine by quadrupole-based ICP-MS
Rapid Comm. Mass Spectrom. **32** (2018), 149-158
DOI: 10.1002/rcm.8018
25. A. Kuklya, L. Coban, F. Uteschil, K. Kerpen, U. Telgheder:
Direct inlet probe ion mobility spectrometry.
Talanta **180** (2018) 61-68
DOI:10.1016/j.talanta.2017.12.028
26. H. L. Wiegand, K. Kerpen, H. V. Lutze, T. C. Schmidt:
Response to Comment on "investigation of the Iron-Peroxo Complex in the Fenton Reaction: Kinetic Indication, Decay Kinetics, and Hydroxyl Radical Yields"
Environ. Sci. Technol. **52(7)** (2018), 4483-4484
27. H. V. Lutze, M. Koti, J. Türk, T. C. Schmidt:
Die Rolle der Realmatrix in der oxidativen Wasseraufbereitung
GWF, Wasser-Abwasser **159(10)** (2018), 10-12

Conferences and Meetings

Organization



Annual Meeting of the Water Chemistry Society, Papenburg, May 07 to 09, 2018

(for more details check <http://www.wasserchemische-gesellschaft.de/de/wasser-2018>)

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 sixth time the annual meeting of the society, this year in Papenburg, a small town in Northwest Germany best known for the Meyer dockyards that produce many of the world's huge cruise ships. The environmental impact of cruises was also the topic of the public lecture on Monday night. On Tuesday the participants could then visit the shipyards, followed by the conference dinner on the premises. More than 280 scientists gathered and discussed for three days 29 oral and 97 poster presentations on all aspects of water chemistry including analytics, micropollutants, and treatment processes. Laura Wiegand of the Schmidt group presented a lecture on the transformation of Bisphenol S in the Fenton system. Dr.-Ing. Eduard Rott, University of Stuttgart was awarded with the Willy-Hager-Preis for his PhD thesis "Investigations of the elimination of phosphor from industry wastewater containing phosphonates". The PhD prize of the Water Chemistry Society was awarded to two outstanding young scientists, Dr. Stefan Bieber, TU Munich, for his thesis "International management strategies for trace organic compounds in waterbodies and supporting advanced analytical techniques" and Dr. Kevin Jewell, University of Koblenz-Landau for his thesis "Investigations of chemically and biologically induced transformation reactions of micropollutants during biological wastewater treatment processes". Finally, Mr. Kurt Böhm, formerly German Chemical Society, received the Water Chemistry Society's badge of honour for his long support of the society in all financial manners and his support in establishing funding for a standardization expert within the Water Chemistry Society.



Drittes Mülheimer Wasseranalytisches Seminar (MWAS) (with IWW), Mülheim, September 12-13, 2018



240 people gathered for the 3rd MWAS in Mülheim for two days to discuss advances in analytical methods in 17 lectures and ca. 30 posters. The accompanying exhibition with 21 companies was sold out already early 2018. The many live demonstrations at the booths and separate company seminars contribute to the special flavor of this meeting that has been co-chaired by Dr. Ulrich Borchers (IWW) and Prof. Torsten Schmidt (UDE-IAC and IWW). In 2018 special emphasis was laid on the one hand on suspect and nontarget screening by high-resolution mass spectrometry and on the other hand on the determination of hygienic parameters.



Analytica conference, Munich, April 11, 2018, Session on “Analysis of Microplastics “

The Water Chemistry Society organizes for many years in the frame of the analytica conference in Munich one or more sessions on current hot topics in water analysis. In 2018, these included two sessions, one on advanced in the analysis of per- and polyfluorinated compounds, chaired by Prof. Christian Zwiener and Dr. Marco Scheurer, the other one by Prof. Torsten Schmidt on the analysis of microplastics. The latter was inspired by a Late Summer Workshop on microplastics organized by the Water Chemistry Society in 2016. The relevance of the topic is underlined by numerous running research projects, including several large projects funded by BMBF. In all of these projects, the further development, standardization and validation of analytical methods is an important part. After an initial overview lecture on the broad topic by Heather Leslie (VU Amsterdam) the currently available analytical methods based on Infrared and Raman spectroscopy, and, as complimentary method, thermoanalysis coupled with GC-MS were presented and discussed. One of the lectures was given by Gerrit Renner, external PhD student in the Schmidt group at the University of Applied Science in Krefeld.

Invited Lectures

T. C. Schmidt, M. Eisinger, C. Freimuth:

Wasserforschung im Ruhrgebiet: Mehrwerte durch Vernetzung von exzellenter Forschung und Praxis
Ministerium für Umwelt, Landwirtschaft, Natur- und Verbraucherschutz NRW: Wasserforschung und
–innovation in NRW - Gemeinsam mehr erreichen?

Oberhausen, November 29, 2018

W. Kaziur, M. A. Jochmann, B. Schilling, T. C. Schmidt:

Automated Microextraction Techniques: Comparison, Optimization and Application in Food Samples
Food Safety Analysis 2018, Singapore, November 28, 2018

T. C. Schmidt, M. A. Jochmann, N. Lorenzo Parodi, W. Kaziur, N. Stojanovic, A. Kremser, J. Laaks:

By failing to prepare, we are preparing to fail - Trends in sample preparation for organic
micropollutants

XIII LASEAC, LATIN AMERICAN SYMPOSIUM ON ENVIRONMENTAL & ANALYTICAL CHEMISTRY, La
Serena, Chile, November 14, 2018 (Plenary Lecture)

H. V. Lutze, J. Terhalle, K. Hupperich, S. Abdi, X. Mutke, I. Schäfer, H. Uhlmann und Torsten Schmidt:
Unerwünschte Transformations- und Nebenprodukte bei der Oxidation: Der Einfluss der
Wassermatrix

Forum Wasseraufbereitung, Karlsruhe, Deutschland, Oktober 31, 2018

H. V. Lutze, J. Terhalle, K. Hupperich, S. Abdi, X. Mutke, I. Schäfer, H. Uhlmann und Torsten Schmidt:
Oxidative transformation processes in aquatic systems, role of matrix components.

W&T-Seminar Eawag, Dübendorf, Schweiz, Oktober 29, 2018

H. V. Lutze, J. Terhalle, K. Hupperich, S. Abdi, X. Mutke, I. Schäfer, H. Uhlmann und Torsten Schmidt
Transformation reactions and the effects of the water matrix

Ecopole 2018, Polanica Zdrój, Poland Oktober 10-13 (Keynote Lecture)

H. V. Lutze

Ozonation in water treatment

Kluge Stunde, Lehrstuhl für Mechanische Verfahrenstechnik, Universität Duisburg-Essen, Duisburg,
September 30, 2018

T. C. Schmidt:

Trends in der Wasseranalytik – wie wird sich das zukünftige Monitoring von organischen
Spurenstoffen verändern?

Annual Meeting Working group Environmental Chemistry and Ecotoxicology in GDCh and SETAC-GLB,
Muenster, September 10, 2018 (Plenary Lecture)

H. V. Lutze

Transformationsreaktionen in wassertechnischen Prozessen

Wissenschaftliches Kolloquium: Wasserressourcen und Hydrochemie- Universität, Stuttgart, Stuttgart, Juli 25, 2018

H. V. Lutze

Transformationsprozesse in aquatischen Systemen

Wissenschaftliches Kolloquium: Umweltanalytik und Schadstoffe, TU Darmstadt, Darmstadt, Juli 4, 2018

T.C. Schmidt, C. Freimuth, M. Eisinger:

Urban water management Between stakeholders and excellent science

Brussels, June 21, 2018, "Grand Challenges: Answers from North Rhine-Westphalia "Sustainable urban water management - prepared for the future"

M. A. Jochmann, B. Schilling, W. Kaziur, T. C. Schmidt

In-Tube Extraction: Optimization Strategies and Applications in Food and Environmental Science
42nd International Symposium on Capillary Chromatography, Riva del Garda, May 18, 2018

T. C. Schmidt, N. Stojanovic, M. Blessing, M. A. Jochmann:

The Quest for Isotope Integrity in Compound-Specific Stable Isotope Analysis

42nd International Symposium on Capillary Chromatography, Riva del Garda, May 16, 2018

T. C. Schmidt, M. A. Jochmann, L. Zhang, D. M. Kujawinski, J.-B. Wolbert, E. Federherr, S. Willach, D. Köster, N. Stojanovic:

What Stable Isotopes can tell us about the world: From prehistoric times to current doping scandals
TU Graz, Chemistry Colloquium, March 07, 2018

Institute Colloquium

22.01.2018	<p>Prof. Dr. Jules Griffin, Department of Biochemistry, University of Cambridge</p> <p>From 5000 people to 50 μm: studying fatty liver disease using high resolution mass spectrometry</p>
29.01.2018	<p>Dr. Jochen Türk, IUTA</p> <p>Instrumentelle und wirkungsbezogene Analytik bei der erweiterten Abwasserreinigung zur Spurenstoffelimination</p>
23.04.2018	<p>Dr. Michael Maiwald, Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin</p> <p>Aktuelle Herausforderungen für die Prozessanalytik – von der Online-NMR-Spektroskopie im Feld bis zum Plasmaspektrometer auf dem Acker</p>
28.05.2018	<p>Prof. Dr. Martin Elsner, TU Munich</p> <p>Advancements in Compound-specific Isotope Analysis (CSIA): Perspectives for Studying Reaction Mechanisms in Complex Systems</p>
01.06.2018	<p>Prof. Dr. Jin-Ming Lin, Tsinghua University, China</p> <p>Droplet Generation for Cell Analysis on Microfluidics and Mass Spectrometry</p>
02.07.2018	<p>PD Dr. Bernd Kammerer, Uni Freiburg</p> <p>Massenspektrometrische Metabolomanalysen in der medizinischen Forschung</p>
08.10.2018	<p>Hans-Gerd Janssen, Unilever and University of Amsterdam, NL</p> <p>Optimization of Column Formats and Flow Conditions in Comprehensive GC\timesGC</p>
03.12.2018	<p>Karl Speer, TU Dresden</p> <p>Authentizität von Sortenhonigen</p>

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.



WissensNacht Ruhr 2018, 28. September 2018 „Wasserwelt“, Hochschule Ruhr West - Campus Mülheim an der Ruhr

How do you get dirty water clean again? Why is the candle floating, but the diver is sinking? How do I make pictures of sugar, color and water? And is red cabbage really rainbow colored?



The IWW Center for Water, in cooperation with the Department of Instrumental Analytical Chemistry (Dr. Ursula Telgheder and Claudia Ullrich), has offered two interactive stations, one for water purification and one with various small experiments. During the water purification, visitors were given a natural sample that they could treat using different levels of purification, just as they do with real wastewater. The hands-on experiments were independent and especially interesting for 'smaller' visitors. Here they could learn about salt content, refractive index and many other properties of water in a playful way.

Trial Course of Studies (Probestudium Chemie), 12.12.2017 “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 and Claudia Ullrich 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



Liana Ava AbdiGhahroudi, 5 July 2018

Weddings



Sasho and Myrto Joksimoski, 22 September 2018

Picture Galleries

Future Water – Zweite Fortschrittswerkstatt Wasser (24 Jan 2018)



Birthday Celebration Prof. Dr. Torsten C. Schmidt (22.05.2018)



Celebration Party „100 Years Analytical Chemistry“ (06 Jul 2018)





Works Outing Trip to Bad Marienberg (14 Sep 2018)





