Institute of Hydrochemistry
Department of Chemistry
Technical University of Munich

Annual Report 2018

Institute of Hydrochemistry
Chair of Analytical Chemistry and Water Chemistry

Technical University Munich
Chair of Analytical Chemistry and Water Chemistry
Marchioninistraße 17
81377 München
Tel: +49 89 2180-78232
Fax: +49 89 2180-78255
www.hydrochemistry.tum.de

Members of the Institute of Water Chemistry (IWC) in December 2018

Contents

Research

Dear friends and colleagues,

"*the only thing that is constant is change*". Heraclitus must have thought of the Institute of Hydrochemistry (IWC) - so well does the quote describe these exciting, but also challenging times. The move of everyone into the new laboratories at Garching is still held off by rectification work. An advance party of the Isotope Group is already commuting between Garching and the Helmholtz Center in Neuherberg, while the Hydrogeology group is in transition to the TUM center to join the Chair of Hydrogeology and build bridges within the Water Cluster. Under these circumstances I am proud that we have managed to keep up what we are best at: advancing scientific analytical solutions to important environmental questions.

- "Why are organic micropollutants (pesticides, pharmaceuticals) so persistent?" – In an ERC project in the Isotope Group we discovered the relevance of mass transfer at low pollutant levels. Bioavailability limitation appears to be the trigger for physiological adaptation that puts a limit to biodegradation when concentrations become low. Innovative approaches will, therefore, be needed to overcome intrinsic limitations in the bioremediation of trace pollutants.

- "How can we beat time in the diagnosis of pathogens?" Culture-base methods are slow when it comes to identifying pathogenic genotypes of *Legionellae*. With a novel viability haRPA assay the Bioanalytics Group offers a chance to be fast from now on: culture-based methods can be replaced in the future for the monitoring of engineered water systems like in the case of *Legionallae* outbreaks in condensation recooling plants.

- "How persistent is microplastics?" While the Raman Group is pushing boundaries of Raman microspectroscopy to advancing reliable protocols of micro- and nanoplastics analysis, a newly acquired DFG project already aims to take the next step: these advances will be combined with stable isotope Raman microspectroscopy and surface enhanced Raman scattering to investigate microbial degradation of plastics at the single cell level. Congratulations, Natascha!

- “What’s sorbed on exhaust particles?” In times when most public attention is directed at NOx, the Laser Group is targeting particles as even more health-relevant topic. Together with colleagues from the TUM spin-off company Plasmion GmbH, and with support of the EU project Down-to-Ten, a new HEILOS/SICRIT/MS (plasma discharge) system is harvested to characterize volatile coatings on aerosol particles, producing unprecedented insights into automotive exhaust composition.

Last but not least, I look forward to announcing an upcoming highlight: on July 7th to 12th 2019 we will be hosting the biannual cross-disciplinary ISOTOPES conference at the TUM center in Raitenhaslach. Chemists, enyzymologists, theoreticians, analytical chemists and biogeochemists will exchange latest trends in the measurements of isotope effects and their interpretation to advance the investigation of environmental processes.

I would like to conclude by thanking all members of the institute for their work and dedication in times of change – and by our friends for their continued support. I look forward to the next year with you!

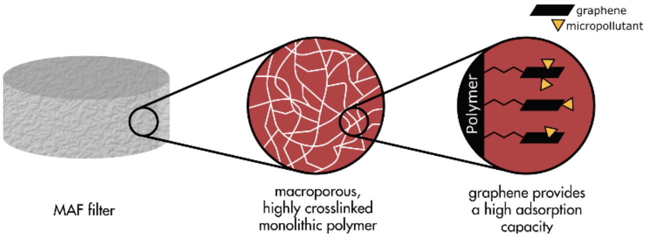
Kind wishes,
Martin Elsner

Graphene-Modified Polymer Monoliths for High Throughput Extraction of Micropollutants for Compound-Specific Isotope Analysis

Application of Compound-specific isotope analysis (CSIA) to field studies is still limited due to low environmental concentrations of micropollutants. First experiments indicate the suitability of graphene-modified polymer monoliths for an enrichment of large-volume water samples within feasible timescales.

State of the Art. Compound-specific isotope analysis has been demonstrated to be highly suitable for the evaluation of transformation processes of micropollutants in laboratory experiments. However, analytical challenges associated with low micropollutant concentrations (sub-µg/L range) in environmental water samples still limit applicability of CSIA approach to field studies due to large volumes of water necessary for extraction. Since conventional solid-phase extraction techniques often fail in processing large volumes in feasible timespans, a high throughput concept for extraction is needed.

Analytical Approach. Monolith adsorption filters (MAF) offer a promising solution to process large volumes of water in reasonable time (i.e. up to 1000 mL/min). MAFs are epoxy-based polymers prepared by self-polymerization of polyglycerol-3-glycidyl ether in organic solvent as porogene. A highly cross-linked structure with high porosity (79%) and large pores (i.e. from 15 to 25 µm) enables high throughput of liquid samples. We explored the use of graphene oxide to modify the MAFs surface chemistry in order to enable pi-pi electron donor-acceptor interactions with the micropollutants.



Schematic illustration of a graphene-modified monolithic adsorption filter (MAF).

Results. Amine groups were successfully immobilized onto the pore surface via the reaction of epoxide groups with the polyetheramine Jeffamine. Subsequently, graphene oxide (GO) was covalently attached by coupling the amine groups using dicyclohexylcarbodiimide as a coupling agent. MAFs functionalized with reduced graphene oxide (rGO) were then obtained via chemical reduction by ascorbic acid. Sorption experiments with rGO-modified MAFs as well as bulk GO and rGO revealed that rGO exhibits higher sorption capacity towards selected pesticides (chloridazon, isoproturon, terbuthylazine, s-metolachlor) by factors 1.8 to 5.5. First results show the suitability of rGO for modification of MAFs surface chemistry.

David Glöckler, Rani Bakkour

References

(1) Elsner, M., Imfeld, G., Compound-specific isotope analysis (CSIA) of micropollutants in the environment — current developments and future challenges. Curr. Opin. Biotech. 2016, 41, 60-72.

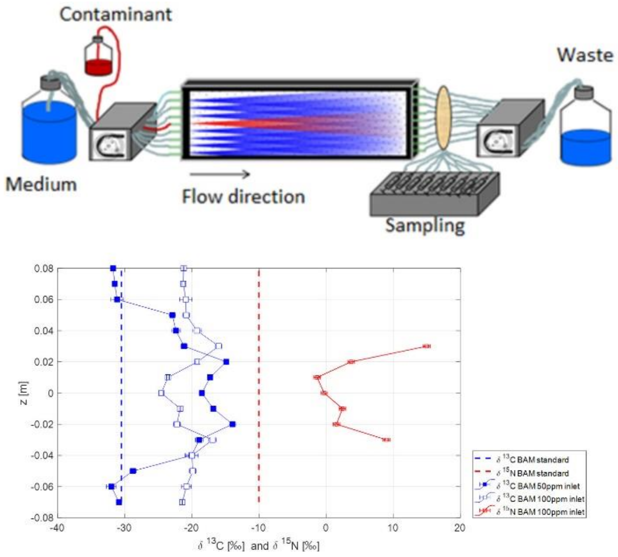
(2) Peskoller, C., Niessner, R., Seidel, M., Development of an epoxy-based monolith used for the affinity capturing of Eschericha coli bacteria. J. Chromatogr. A. 2009, 1216, 3794-3801.

Funding
DFG - CRC CAMPOS

Compound-specific stable-isotope analysis (CSIA) of micropollutants to explore bioavailability in tank experiments

Bioavailability limitation is a putative bottleneck for micropollutant biodegradation in groundwater. Decreasing concentrations in the gradient of a sediment tank were used to explore whether compound-specific isotope fractionation disappears at low levels providing direct evidence of bioavailability limitations.

State of the Art. Recent batch and chemostat experiments used compound-specific stable isotope analysis (CSIA) to highlight mass transfer limitations as barrier for micropollutant biodegradation at low concentrations [1-3]. Analogous evidence is currently missing in groundwater model systems.



Two-dimensional sediment tank experiment setup and C and N isotope values measured alone the outlet boundary of the tank in the biotic experiment.

Experimental Setup. A two-dimensional sediment tank experiment served to mimic groundwater. A solution of 2,6- dichlorobenzamide (BAM) was continuously injected into the center port of the tank to establish a plume with a gradient of high to low concentrations by transverse dispersion. Samples were taken at different ports to probe for the vertical gradient of concentrations, biomass, isotope values etc at the end of the tank.

Results. Experiments in the absence of degrader organisms demonstrated that hydrodynamic dispersion did not affect observable $^{13}C/^{12}C$ and $^{15}N/^{14}N$ isotope values. Subsequent biotic experiments showed that inoculation with *Aminobacter* MSH1 induced BAM biodegradation. Degradation-associated isotope fractionation of BAM was highest in the fringes of the plume where O_2 and BAM mixed. In contrast, fractionation declined towards the top and the bottom where BAM concentrations were lowest and most complete degradation would be expected. We hypothesize that this reflects a masking of degradation-induced isotope fractionation by mass transfer limitations. Hence, we obtained evidence of bioavailability limitation during biodegradation specifically at low concentrations.

Fengchao Sun

References

(1) Ehrl, B., Gharasoo, M., Elsner, M., Isotope fractionation pinpoints membrane permeability as a barrier to atrazine biodegradation in gram-negative Polaromonas sp. Nea-C. Environ Sci Technol.2018, 52(7),4137-4144, DOI: 10.1021/acs.est.7b06599

(2) Ehrl B., Kundu, K., Gharasoo, M., Marozava, S., Elsner, M., Rate-Limiting Mass Transfer in Micropollutant Degradation Revealed by Isotope Fractionation in Chemostat, Environ. Sci. Technol. 2018 53, 1197–1205, DOI: 10.1021/acs.est.8b05175

(3) Gharasoo, M., Ehrl, B., Cirpka, O., Elsner, M., Modeling of contaminant biodegradation and compound-specific isotope fractionation in chemostats at low dilution rates, Environ. Sci. Technol. 53 (2019) 1186–1196, DOI: 10.1021/acs.est.8b02498

Funding

European Research Council Consolidator Grant - Grant number 616861

Cooperation

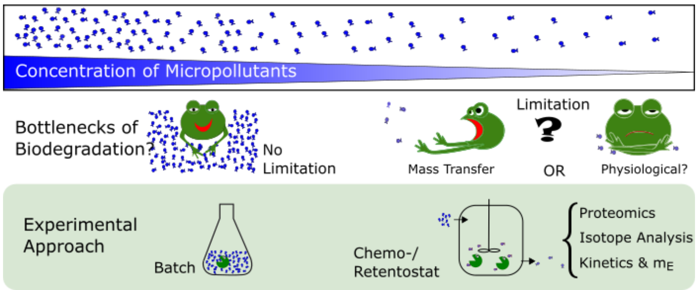
Prof Olaf Cirpka
Dr. Martin Thullner

Observing the onset of limitations for micropollutant biodegradation at low concentrations

Drinking water resources are contaminated by man-made chemical contaminants such as pesticides. Can we observe why natural micropollutant degradation is limited at low concentrations?

State of the Art. Biodegradation of anthropogenic chemicals often slows-down at low concentrations. Consequently, chemical micropollutants are found in ground- and surface water at concentrations that are low, but still exceed drinking water thresholds (0.1 μg L^{-1}) [1]. Two particular drivers are debated to cause limited degradation: (i) mass-transfer limitation(uptake into microbial cells); or (ii) physiological adaptation meaning that microorganisms switch to maintenance mode and down-regulate enzyme activity when - below a certain low concentration - extensive degradation appears to be no longer energetically favorable. Conventional degradation studies at high (mg L^{-1}) concentrations cannot highlight the limiting factors at low concentrations.

Experimental Approach. *Arthrobacter aurescens* TC1 was cultivated in chemostats and retentostats to study degradation of the persistent herbicide atrazine at different steady-state concentrations (12-440 μg L^{-1}). A combination of compound-specific isotope fractionation analysis (CSIA) and proteomics explored limiting factors directly at low concentrations.



Identifying the bottleneck of degradation at low concentrations using a multi-disciplinary approach in chemostat and retentostats.

Results. At higher concentrations (82-440 μg L^{-1}) degradation-associated isotope fractionaton (ε^{13}C) fully represented the isotope effect of the enzymatic reaction. At lower concentrations (30-60 μg L^{-1}) contrasting, smaller ε^{13}C indicated that mass transfer across the cell membrane became rate-limiting [2]. Retentostat cultivation at 12μg L^{-1} resulted in complete mass-transfer limitation evidenced by the disappearance of ε^{13}C. Simultaneous physiological adaptation was reflected in low protein turnover, a change in morphology and a reduction of the energy requirement for maintaining the viability (m$_E$). The results indicate that mass-transfer limitation was a trigger for bacterial adaptation and that together mass transfer limitation and bacterial adaptation slowed degradation of micropollutants at low concentrations.

Kankana Kundu, Sviatlana Marozava, Benno Ehrl

References

1. *Fenner K, Canonica S, Wackett LP, Elsner M. Evaluating pesticide degradation in the environment: blind spots and emerging opportunities. Science 2013; 341: 752–758, DOI:10.1126/science.1236281*
2. *Ehrl BN, Kundu K, Gharasoo M, Marozava S, Elsner M. Rate-Limiting Mass Transfer in Micropollutant Degradation Revealed by Isotope Fractionation in Chemostat. Environ. Sci. Technol. 2019, 53:* 1197–1205, DOI: 10.1021/acs.est.8b05175*.*

Funding

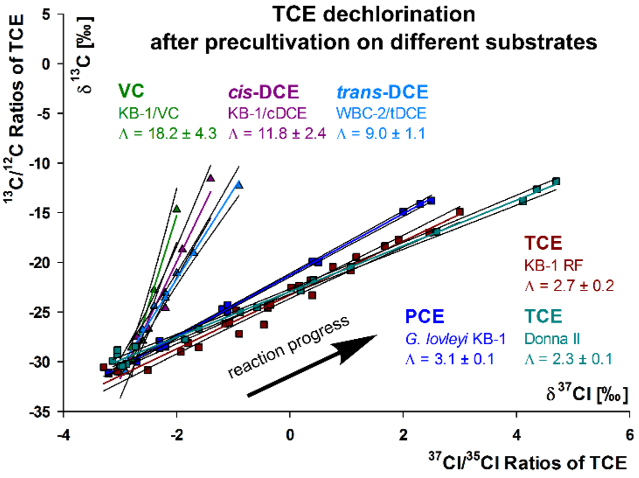
European Research Council Consolidator Grant - Grant number 616861

Mechanistic dichotomy in bacterial trichloroethene dechlorination revealed by carbon and chlorine isotope effects

Chlorinated ethenes are toxic pollutants that threaten groundwater quality. Dual element isotope analysis revealed different underlying dehalogenation mechanisms for bacterial cultures and provided a plausible mechanistic explanation for the different degradability of TCE vs. *cis*-DCE at contaminated sites.

State of the Art. Trichloroethene (TCE) can be reductively dehalogenated to harmless ethene by specialist microorganisms, particularly *Dehalococcoides*. However, the reaction mechanisms in reductive dehalogenase enzymes (RDases) have remained elusive. Furthermore, reductive dehalogenation often stops at toxic *cis*-1,2-dichloroethene (*cis*-DCE) or vinyl chloride (VC). Our aim was to study the differences in *cis*-DCE and TCE microbial dechlorination and to explore the influence of culturing conditions and associated enzymes on TCE dechlorination mechanisms.

Analytical Approach. Compound-specific carbon ($\delta^{13}C$) and chlorine ($\delta^{37}Cl$) isotope fractionation of TCE and *cis*-DCE was measured in pure and mixed bacterial, organohalide-respiring, cultures. The magnitude of carbon relative to chlorine isotope effects, as expressed by the slope Λ of $\delta^{13}C$ vs. $\delta^{37}Cl$ regressions, was used to distinguish different reaction mechanisms.



Different trends of TCE dechlorination.

Results. The slope Λ was larger in the transformation of *cis*-DCE by two *Dehalococcoides mccartyi* strains compared to TCE transformation by *Geobacter lovleyi* strain KB-1. Λ was also larger for TCE transformation for cultures that had been precultivated on lesser chlorinated ethenes (*cis*-DCE, *trans*-DCE, VC). Λ slopes of precultivated cultures match reported values for cob(I)alamin addition followed by protonation, whereas Λ values for TCE-adapted cultures match values for cob(I)alamin addition followed by chloride elimination. These contrasting trends demonstrate the existence of distinct reductive dechlorination mechanisms, for specific substrates (*cis*-DCE vs. TCE), and for the same substrate (TCE) in cultures preconditioned for different substrate utilization. This mechanistic dichotomy indicates that RDases and their reaction chemistry are tailored to chemical target structures and may provide an answer to why chlorinated ethene remediation frequently stalls at *cis*-DCE[1].

Christina Lihl, Alfredo Pérez-de-Mora, Armin H. Meyer, Martina Daubmeier

Reference

(1) Lihl, C.; Douglas, L.M.; Franke, S.; Pèrez-de-Mora, A.; Meyer, A.H.; Daubmeier, M.; Edwards, E.A.; Nijenhuis, I.; Sherwood Lollar, B.; Elsner, M.: Mechanistic dichotomy in bacterial trichloroethene dechlorination revealed by carbon and chlorine isotope effects. Environ. Sci. Technol. 2019, in press

Funding

SNF – Swiss National Science Foundation

Cooperation

University of Toronto – Barbara Sherwood Lollar, Lisa Douglas and Elizabeth Edwards

UFZ Leipzig – Ivonne Nijenhuis and Steffi Franke

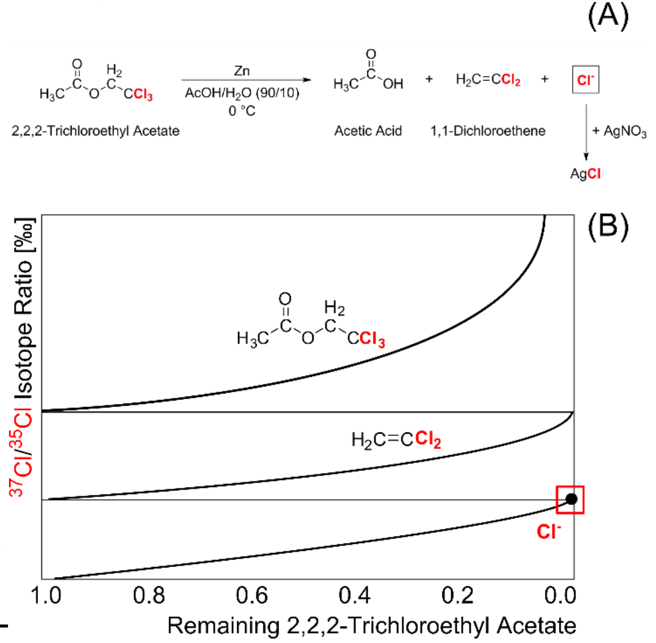
Synthesis and characterization of a calibration standard for stable chlorine isotope analysis

Compound-specific stable isotope analysis of chlorine is an important tool in environmental chemistry. By using organic chemistry a laboratory standard for isotopic characterization was synthesized.

State of the Art. For achieving a good accuracy during stable isotope analysis of chlorine, isotope standards are crucial to be run in parallel with samples. Specifically, it is recommended to use two standards which bracket the isotope values of the samples. For chlorine a few international standards are available, but all of them show very similar isotope values near 0 ‰. Only one standard, USGS38, shows an isotopic shift (-87.9 ‰), but is of limited availability and very expensive. Thus, working standards for daily chlorine isotope analysis are often characterized against only one international standard. A second readily available standard with an isotopic shift for characterization is needed.

Analytical Approach. 2,2,2-Trichloroethyl acetate was used as starting material. As depicted in panel A of the Figure, the trichloroethyl group was removed via reductive elimination under reflux conditions. After stopping the reaction, silver nitrate solution was added to precipitate the formed chloride as silver chloride. For characterization via GC-IRMS and GC-ICP-MC-MS the international standards ISL-354 ($\delta^{37}Cl$ = +0.05 ±0.03 ‰) and USGS38 ($\delta^{37}Cl$ = -87.90 ±0.24 ‰) were used. Prior to characterization all substances were converted to methyl chloride.

Results. Conversion of 2,2,2-trichloroethyl acetate produced pure silver chloride which was named “CT16”. The results of the characterization via GC-IRMS and GC-ICP-MC-MS were in accordance with each other. The mean value over all measurements, $\delta^{37}Cl_{CT16}$ = -26.82 ±0.18 ‰ (n = 16), is considered as the true value. This value shows a relatively large shift when compared to most international chlorine isotope standards. This can be explained by the intramolecular chlorine isotope effect during reductive elimination according to panel B in the Figure. The large difference will be of great advantage in future chlorine standards characterization: Calibration against two different isotope standards will improve the precision and the trueness of working standards which will consequently also improve the precision and trueness of daily chlorine isotope analysis.



(A) Synthesis of the silver chloride standard CT16 via reductive elimination and subsequent precipitation with $AgNO_3$. (B) Expected intramolecular isotope fractionation and resultant strategy to recover produced chloride with pronounced changes in chlorine isotope values.

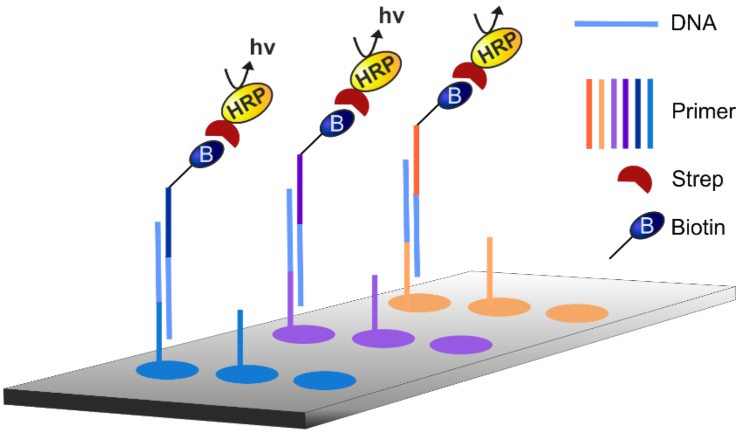
Christina Lihl, Heide K.V. Schürner, Martina Daubmeier, Benjamin Heckel, Aileen Melsbach

Funding
SNF – Swiss National Science Foundation

Cooperation
UFZ Leipzig – Julian Renpenning, Matthias Gehre

DNA microarray for detection of pathogens and antibiotic resistance gene *bla*$_{\text{CTX-M}}$ in surface water

Antibiotic resistance is a problem for treatment of infections worldwide. In surface water, antibiotic resistant bacteria are also present and need to be monitored to assess potential risks and dissemination pathways. Using the developed DNA microarray, we are able to detect pathogenic bacterial species and the widely distributed resistance gene *bla*$_{\text{CTX-M}}$.



Schematic overview of a nucleic acid amplification test on chemiluminescence DNA microarrays.

State of the Art. Antibiotic resistant bacteria carry antibiotic resistance genes (ARGs) which are responsible for changes within the bacteria. The current gold standard for detecting antibiotic resistance is cultivation followed by PCR which is time consuming and only feasible for culturable bacteria. In environmental samples, however, non-culturable bacteria make up a larger fraction of the total count.

Analytical Approach. To provide faster results the existing heterogeneous asymmetric recombinase polymerase amplification (haRPA) assay on the microarray chip[1, 2] was adapted for the detection of the ARG *bla*$_{\text{CTX-M}}$, an extended spectrum β-lactamase, as well as for the pathogenic bacteria *Klebsiella pneumoniae* and *Pseudomonas aeruginosa*.

Results. The haRPA for *bla*$_{\text{CTX-M}}$ was compared to an established PCR assay (in collaboration with LGL) showing 100% agreement for detection of *bla*$_{\text{CTX-M}}$ in *Escherichia coli* and *K. pneumoniae*. Detection of *P. aeruginosa* with haRPA was successfully established in singleplex measurements without cross reactivities towards other species. Duplex measurements with detection of one bacterial species (*K. pneumoniae* or *P. aeruginosa*) and the *bla*$_{\text{CTX-M}}$ gene were successfully carried out. First experiments for triplex measurements with both bacterial species and ARG confirmed the proof of principle.

Lisa Göpfert, Michael Seidel

References

(1) A. Kunze; M. Dilcher, A. Abd El Wahed, F. Hufert, R. Niessner, M. Seidel On-chip isothermal nucleic acid amplification on flow-based chemiluminescence microarray analysis platform for the detection of viruses and bacteria. Anal. Chem. 2015, 88, (1), 898–905.

(2) C. Kober, R. Niessner, M. Seidel Quantification of viable and non-viable Legionella spp. by heterogeneous asymmetric recombinase polymerase amplification (haRPA) on a flow-based chemiluminescence microarray. Biosensors and Bioelectronics 2018, 100, 49–55.

Funding

BMBF (Project METAWATER; (FKZ: WU1346A), JPI Water Project)

Cooperation

Bayerisches Landesamt für Gesundheit und Lebensmittelsicherheit (LGL)

Continuous synthesis of PVP stabilized monodispersed gold nanoparticles using flow-based microreactor

Gold nanoparticles were widely used because of excellent properties. In this project, we report an automated tape based microfluidic device for the continuous flow synthesis of stabilized and monodispersed gold nanoparticles.

State of the Art. Gold nanoparticles (Au NPs) have exceptional biocompatibility and possess unique structural, electronic, magnetic, optical, catalytic and molecular recognition properties. Hence GNPs are very attractive for many biological applications. Au NPs synthesis can be done by number of methods. The chemical synthesis by reducing metal salts is a simple process, which requires the mixing of the reagents at well-defined external conditions. The chemical reduction method and the choice of a capping agent depends on variety of parameters that can influence the physical and chemical properties of the resulting particles. To achieve stable nanoparticles with specific size, reaction conditions should be controlled. Therefore, microfluidic reactors with online-detection methods are preferable.[1]

Combined instrument for nanoparticle synthesis with multilayer microreactor

Experimental Approach. In this work, polyvinylpyrrolidone (PVP) capped AuNPs were synthesized in a continuous tap based microfluidic device using ascorbic acid as the reducing agent and tetrachloroaurate(III) ions as the gold precursor. The size was controlled by changing the flow rate and the pH. This approach allows rapid, easy, low cost and automated synthesis of the gold colloidal. The reproducibility, stability, monodispersity and size control will be investigated.

Results. Stabilized gold nanoparticles can be obtained with good reproducibility on microfluidic microreactors. Higher ascorbic acid flow rates increased the dilution effect. As consequence, the synthesis process was dominated by the nucleation which resulted in smaller particles. Ascorbic acid solutions at higher pH possess a stronger reducing power due to its dibasic properties which led to smaller AuNPs. PVP was proved to be the effective stabilizing agent.

Yanwei Wang

References

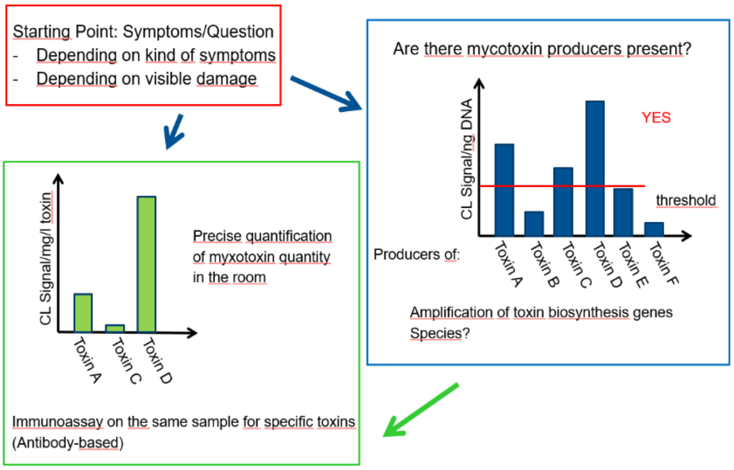
(1) . Bemetz, J.; Wegemann, A.; Saatchi, K.; Haase, A.; Häfeli, U.O.; Niessner, R.; Gleich, B.; Seidel, M. Microfluidic-Based Synthesis of Magnetic Nanoparticles Coupled with Miniaturized NMR for Online Relaxation Studies. Analyt. Chem., 2018, 90, 16, 9975-9982.

Funding
China Scholarship Council

Detection of Mycotoxins and Mycotoxin Producers in Indoor Air

In industrialized countries, a big part of people‘s lives is spent indoors. The problem of indoor mold causing allergies and infections is long known but hardly dealt with. Also, the fact that indoor molds just as food molds can produce very harmful mycotoxins is largely undervalued. Mycotoxins are small volatile secondary metabolites produced by fungi which can cause disease and even death in humans. We aim to develop a rapid and reliable technique for the detection of mycotoxins and their producers. This is especially important for reliable risk analysis in cases like water damages in homes and working places.

State of the Art. To date the most used methods to test for microorganism contamination in indoor air are culture-based or microscopy methods which are relatively inaccurate. Mycotoxins themselves are detected via chromatography or mass spectrometry methods which are very labor intensive and expensive. There is a strong requirement for a cheaper and faster assessment method.



Workflow for the detection of Mycotoxins and their producers

Analytical Approach. The aim of this work is to provide a fast and reliable molecular biological method to specifically detect mycotoxins and their producers amongst indoor air contaminants. For this, an isothermal recombinase polymerase amplification assay[1] and an indirect competitive immunoassay on a chemiluminescence based microarray chip[2] will be developed. In case of supposed fungal contamination, first a DNA based Chip will be used to identify toxin producers, if a producer is present an immunoassay based chip will detect and quantify toxin concentration.

Results. As a proof of principle, we could show that zearalenone producers can be detected by a haRPA on the DNA microarrays.

Katharina Sollweck

References

(1) Kunze, A.; Dilcher, D.; Abd El Wahed, A.; Hufert, F.; Niessner, R.; Seidel, M., On-chip isothermal nucleic acid amplification on flow-based chemiluminescence microarray analysis platform for the detection of viruses and bacteria. Anal. Chem. 2015, 88, (1), 898–905.

(2) Oswald, S.; Karsunke, X. Y. Z.; Dietrich, R.; Märtlbauer, E.; Niessner, R.; Knopp, D., Automated regenerable microarray-based immunoassay for rapid parallel quantification of mycotoxins in cereals. Anal. Bioanal. Chem. 2013, 405, (20), 6405–6415..

Funding
AIF-ZIM

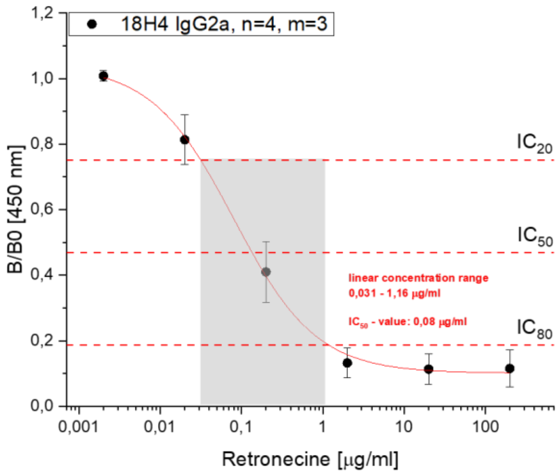
Cooperation
Domatec GmbH

Development of an immunological screening method for the determination of toxicologically relevant pyrrolizidine alkaloids in herbal tea and related matrices

Toxic pyrrolizidine alkaloids (PAs) can be found as contaminants in a wide range of plant-based food sources. Defined limit concentrations for PAs in food are expected to be introduced by the EU near-term. Therefore, food industries require a screening method for cost- and time-effective monitoring of unprocessed plant resources. In this context, bioanalytical methods based on immunological detection of the alkaloids are most suitable.

State of the Art. PAs are so called secondary metabolites and naturally occurring alkaloids. They are produced by 3% of all flowering plants as a defence mechanism against herbivores. Worldwide more than 660 PAs including corresponding N-oxides (PANOs) can be identified. They provide great structural variety and can be metabolized to highly reactive pyrrole esters, which form harmful DNA- and protein adducts. Therefore, contamination of human food sources (e.g. herbal tea) are supposed to give rise to acute or chronic toxicity.

Compared to standard mass spectrometry-based methods, cost- and time- effective antibody-based bioanalytical methods provide parallel processing of many samples and require only minor trained staffing. Therefor the aim of this project is to develop and validate an immunological screening method for the determination of toxicologically relevant PAs (e.g. Retronecine).



Calibration curve mAb 18H4 (linear working range 0,031 – 1,16 µg/ml, IC_{50} = 0,08 µg/ml)

Analytical Approach. Based on the necine base Retronecine, suitable antigens are designed and coupled to protein carriers (BSA or OVA) by using appropriate coupling chemistry. Generated protein conjugates are used for immunization of mice/rats. After hybridoma cell culture, supernatants of single cell clones are screened by direct and indirect competitive ELISAs and most suitable monoclonal antibodies are extensively characterized and used for the immunoassay development.

Results. Based on the screening of cell culture supernatants the most suitable mAb (derived from cell clone 18H4) was extensively characterized and purified for immunoassay development. Finally, plant-based extracts were analysed, and results were validated using LC-MS.

Katharina Zirngibl, Dietmar Knopp

Funding

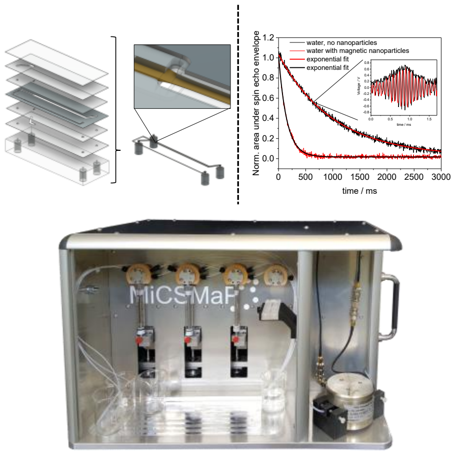
FEI – Research Association of the German Food industry (AiF 19010N)

Cooperation

Prof. Gareis & Dr. Gottschalk, Chair of Food Safety, Veterinary Faculty, Ludwig-Maximilians-University (LMU)

Tape-based Microreactor with Integrated Characterization by T2-Relaxation for Optimization of Synthesis of Magnetic Nanoparticles

Microfluidic syntheses allow controlled and reproducible production of nanomaterials. Coupled with small scale online characterization tools, such systems can be used for fast optimization and production with inline quality control. A system with integrated measurement of NMR relaxation was used for optimization of synthesis conditions of magnetic nanoparticles. Functionalized particles were applied for detection Legionella on porous filters systems after preconcentration.



Explosion view of multilayer microreactor with schematic representation of 3D flow-focusing and experimental setup with integrated pumps and T2-relaxometer.

State of the Art. The use of miniaturized continuous-flow reactors is gaining importance for nanoparticle synthesis, especially for small-scale and decentralized production of nanomaterials. The integration of analytical methods is important for fast synthesis optimization, quality- and process control. However, for the synthesis of magnetic iron oxide nanoparticles systems lack online characterization tools as well as are prone to solid deposition in the microchannels.

Analytical Approach. Magnetic nanoparticles are syn-thesized by a co-precipitation reaction by 3D hydrodynamic flow focusing of an iron salt precursor solution into basic sheath streams in a tape based microreactor. The microreactor is integrated into one machine with pumps and valves for sample handling and a miniaturized nuclear magnetic resonance (NMR) relaxometer for measurement of transverse (T2) relaxation time of hydrogen proton spins in water. The T2 time describes the decay of transverse magnetizations in a static magnetic field after excitation by a radiofrequency pulse and is shortened by the presence of magnetic nanoparticles.

Results. The combined device was used optimize synthesis conditions for maximum T2 relaxivity for higher sensitivity in analytical applications. Synthesized nanoparticles were further coated and functionalized with antibodies. They were applied for labelling and detection of Legionella inside porous filters for the elution free concentration and detection by the same NMR system.

Jonas Bemetz

References

(1) Bemetz, J.; Wegemann, A.; Saatchi, K.; Haase, A.; Häfeli, U. O., Niessner, R.; Gleich, B.; Seidel, M., Microfluidic-Based Synthesis of Magnetic Nanoparticles Coupled with Miniaturized NMR for Online Relaxation Studies. Anal. Chem. 2018, 90, (16), 9975-9982.

Funding

International Graduate School of Science and Engineering (IGSSE), TUM

Cooperation

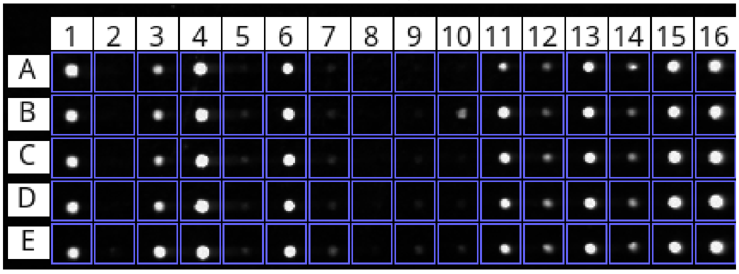
Dr.-Ing. Bernhard Gleich, Munich School of BioEngineering (MSB), TUM

LegioTyper: Automated microarray-based immune-assay for rapid serotyping of *L. pneumophila*

In case of a Legionellosis outbreak source of an outbreak needs to be found promptly to prevent further diseases. Our antibody-based serotyping of *Legionella pneumophila* Sg 1 is able to identify serotypes of *L. pneumophila* in water and its antigens in patients´urine samples within 34 min.

State of the Art. Increasing numbers of legionellosis cases have shown that an innovative, fast and sensitive serotyping method of *L. pneumophila* in water and urine samples is still needed. Cultivation, as gold standard method, takes 10 days and only detects culturable *Legionella* spp. Further methods are applied to type *Legionella* colonies, esp. *L. pneumophila* Sg 1 - 15 as legionellosis is mostly caused by the species *L. pneumophila* (90%).

Analytical Approach. A chemiluminescence sandwich microarray immunoassay (CL-SMIA) was established based on the Dresden panel to detect and serotype all *L. pneumophila* Sg 1 subgroups directly in liquid samples on the new microarray test device MCR-R[1]. A rapid and multiplexed serotyping is possible within 34 min with a panel of 10 sensitive antibodies. A cost-effective polycarbonate microarray chip was implemented to optimize the manufacturing process[2].



Chemiluminescence chip image of a measurement with process water containing L. pneumophila Sg 1, strain Philadelphia-1.

Results. In the last period of the LegioTyper project (www.legiotyper.de) the concentrations of all capture antibodies was adjusted to maximum specific signal and least cross-reactivity. Different sample types like urine and process water were analysed successfully with the established panel. A direct and rapid comparison of patient's urine samples with environmental water samples of putative outbreak sources can be done to rapidly exclude environmental samples for further analytical methods to focus on a smaller number of samples during outbreak investigations.

Catharina Kober

References

(1) Wunderlich, A.; Torggler, C.; Elsaesser, D.; Lück, C.; Niessner, R.; Seidel, M., Rapid quantification method for Legionella pneumophila in surface water. Analyt. Bioanal. Chem. 2016, 408(9), 2203-2213.

(2) J. Bemetz, C. Kober, V. Meyer, R. Niessner, M. Seidel (2019) Succinylated Jeffamine ED-2003 coated polycarbonate chips for low-cost analytical microarrays. Anal. Bioanal. Chem. accepted.

Funding

Bundesministerium für Bildung und Forschung (FKZ: 13N13698)

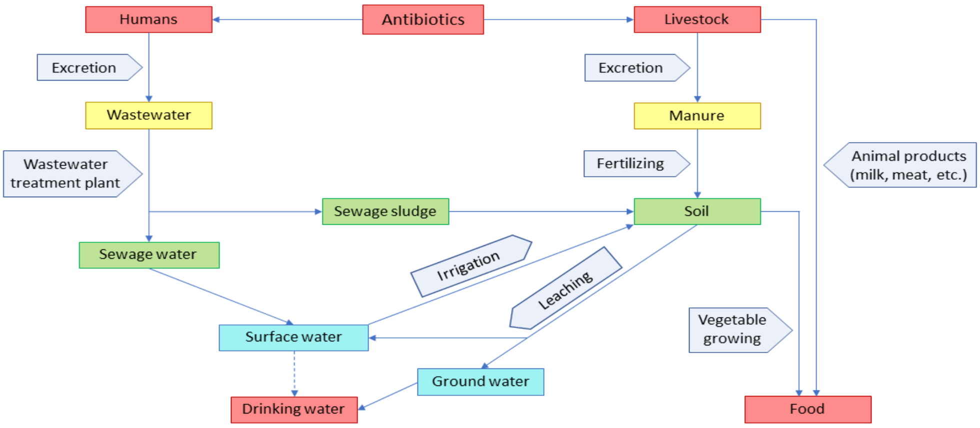
Cooperation

Occupational and Environmental Health, Epidemiology, Bavarian Health and Food Safety Authority, Institute of Medical Microbiology and Hygiene, Institute of Virology, Medical Faculty "C. G. Carus", Technical University of Dresden
GWK Präzisionstechnik GmbH

Detection of antibiotics in liquid matrices by regenerable chemiluminescence microarray immunochips

Antibiotics are increasingly enriched in the ecosystem, and due to their impact on the development of bacterial resistances, they have to be monitored. The established regenerable chemiluminescence microarray immunoassay allows the screening of various antibiotics in a single run. The detection limits can be further reduced by preceding SPE.

State of the Art. Antibiotics are widely used in both human and veterinary medicine. Via wastewater and manure, they are dispensed to the environment and may end up in drinking water and food. The presence of antibiotics induces the development of resistance genes in bacteria. Therefore, a fast and cost-effective multi-antibiotic screening method for the monitoring of both animal products (e.g. milk) and environmental waters is required.



Distribution pathways of antibiotics used in human and veterinary medicine.

Analytical Approach. By means of the automated flow-through analysis platform MCR 3 (GWK Präzisionstechnik, Munich), we have already established a regenerable indirect competitive chemiluminescence microarray immunoassay for the simultaneous detection of various antibiotics, e.g. sulfonamides and β-lactams, in liquid matrices (milk, urine, surface water).

Results. Calibration experiments were carried out for seven sulfonamides. The most sensitive assay was achieved for sulfamethoxazole with a detection limit of 0.1 µg/L. To cover the even lower concentrations of real environmental water samples, a pre-concentration SPE method using Oasis® HLB cartridges (Waters, Milford, CT, USA) is being developed.

Verena Meyer

References

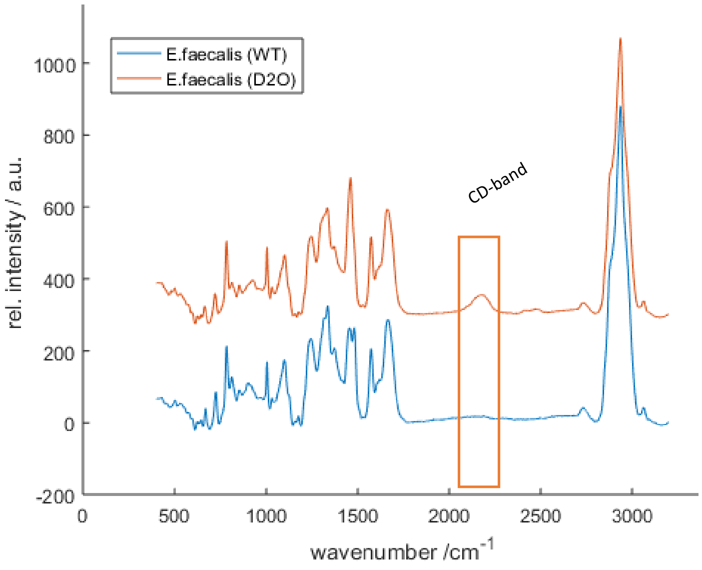
(1) Meyer, V.K.; Meloni, D.; Olivo, F.; Märtlbauer, E.; Dietrich, R.; Niessner, R.; Seidel, M., Validation procedure for multiplex antibiotic immunoassays using flow-based chemilumines-cence microarrays. In: M. Uttamchandani & S.Q. Yao, Small Molecule Microarrays: Methods and Protocols of the series Methods in Molecular Biology, 2017, Volume 1518, 195-212.

Funding
Hanns-Seidel-Stiftung

Monitoring Deuterium Incorporation by Raman Spectroscopy: A Fast Antibiotic Susceptibility Test

Incorporation of deuterium in organisms can easily be monitored by Raman spectroscopy due to the development of a new Raman band. It is the CD stretching vibration which evolves in the else empty region of the Raman spectrum. Thus it allows for easy and fast viability testing of cells and microorganisms. In this project its potential and limit is investigated to develop a fast and reliable Antibiotic Susceptibility Test.

State of the Art. Most established Antibiotic Susceptibility Tests (AST) rely on optical detection of growth inhibition in presence of the drug. Thus it takes several duplication cycles and a minimum time of 8 hours to obtain a profound result by a disc diffusion or broth dilution test which are the two gold standards for AST.



Raman spectra of Enterococcus faecalis. Bottom: wildtype, top: after incubation with D_2O.

Analytical Approach. Confocal microscopy in combination with Raman spectroscopy allows for investigation of whole single cells. The obtained spectrum can be used to identify bacteria down to the strain level and at the same time it depicts their molecular composition. Latter can be used to monitor metabolic activity due to deuterium incorporation and the regarding new CD stretching vibration band at 2050 – 2275 cm^{-1} as can be seen in the spectra of *E. faecalis* on the right side.

Results. In the major part of this project experiments were carried out to proof the good usability of this method for viability studies of Gram-positive and -negative bacteria and a standard protocol to carry out an AST was developed. This was done using three typical antibiotics and tested with reference bacteria and clinical isolates. Thus successful identification of susceptible and resistant specimen was obtained after down to 2.5 hours.

David Bauer

Funding
DFG

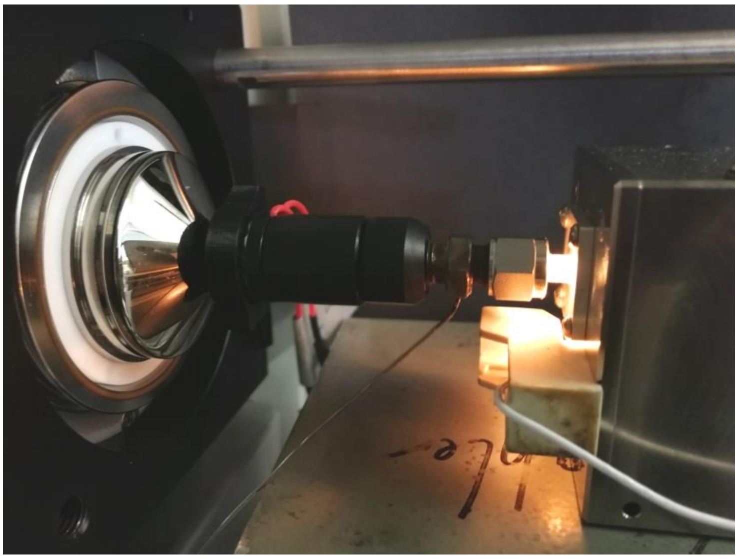
Cooperation
Prof. Stief, Urologische Klinik der LMU München;

PD Dr. Wieser, Max von Pettenkofer-Institut, LMU

Down to Ten - Characterization of Combustion Engine Exhaust Particles in the Size Range from 10 to 23 nm

Nanoparticles emitted from combustion engines are considered a significant health issue. While current legislation limits number of particles larger than 23 nm emitted from vehicles, knowledge about even smaller particles is sparse. Development of new measurement techniques for such small particles is necessary. Our approach includes the use of a mass spectrometer in combination with an aerosol evaporation system and an ionization source based on atmospheric plasma.

State of the Art. DownToTen seeks to develop a reliable and robust methodology to enhance the regulatory approach in the assessment of particle number emissions in the sub 23 nm region (down to at least 10 nm), focusing on state-of-the-art automotive powertrains with direct injection gasoline engines, but also diesel engines, under real-world operation conditions. To this end, DownToTen will first investigate and quantitatively describe the nature and the characteristics of nanoparticles <23 nm (formation, origin, physical and chemical characteristics), and will set up a synthetic aerosol bench for fundamental studies at instrument level for the facilitation of metrology and evaluation purposes. Existing, proposed and under development instruments will be evaluated against rigorous criteria for the measurement of sub-23 nm particles, with emphasis on their applicability as portable emissions systems (PEMS).


MS inlet with SICRIT ionization source and aerosol evaporation system HELIOS.

Results. For off-line chemical characterization of sub-23 nm particles several methods have been tested: Inductively coupled plasma mass spectrometry (ICP-MS), total reflection x-ray fluorescence (TXRF) or neutron activation analysis (NAA). Very little sample amount is challenging for all used methods and the appropriate filter material is of crucial importance. However, artefact-free sampling of nanoparticles is a challenge; hence, we also employ online analytical techniques, which are developed within the framework of the project. Mass spectrometry with a new ionization source from Plasmion, a high-tech start-up company founded by alumni J.-C. Wolf, allows for direct online analysis of exhaust gas. It is combined with particle size fractionation and evaporation systems, thus allowing for the characterization of volatile and semi-volatile particles. The complete system is portable and has been used at measurement campaigns in Finnland.

Klemens M. Thaler

Funding

European Union H2020

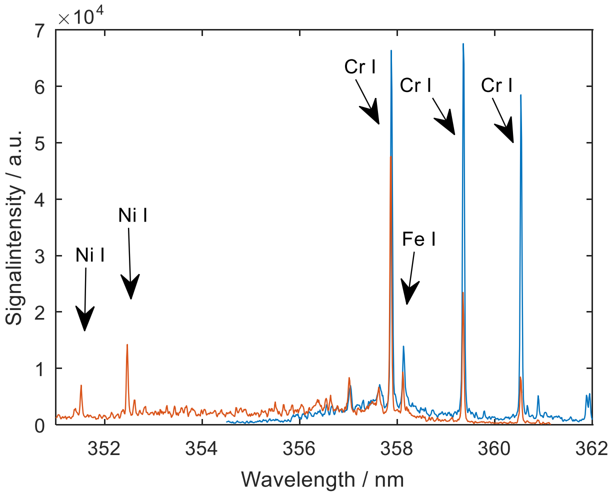
Cooperation

Aristotle University of Thessaloniki, AVL List GmbH, Ricardo UK Ltd, Tampere University of Technology, Graz University of Technology, Joint Research Center, Centro Ricerche FIAT

Laser-Induced Breakdown Spectroscopy (LIBS) for the Analysis of Aerosols

Nano-particle emissions constitute the majority of particulate emissions from exhaust and are especially harmful for human health. LIBS allows for on-line determination of elemental composition of such aerosols.

State of the Art. Ultrafine particles (diameter < 100 nm) are produced by combustion engines, break wear, and industrial processes. Current analytical methods for elemental analysis of such aerosols need time consuming sample collection on filters. So far, LIBS has been used for the on-line elemental analysis of aerosols with larger particles.



LIBS-spectrum of a CrNi-steel aerosol.

Analytical Approach. The beam of a pulsed Nd:YAG-laser is focused into an aerosol stream to produce a plasma. The emitted light is analyzed with an echelle spectrometer equipped with a gated detector.

Results. A LIBS setup was developed and tested with different model aerosols (Cu, Fe, Al, Ni, Cr). Within the first microsecond after the laser pulse continuum light and ionic lines dominate the emission. Later also atomic lines and molecular bands can be detected. Experiments on the temporal behavior of the emitted light were performed to optimize gating of the detector for differentiation between continuum background and analyte signal. After optimization particles with diameters down to 32 nm could be measured. Limits of detection between 7.7 µg m^{-3} (Cu) and 3.5 mg m^{-3} (Fe) were achieved with a measurement time of 75 s. Simultaneous measurement of multiple elements is also possible as shown in the figure. For further improvement of the sensitivity an aerodynamic lens for the focusing of particles with diameters between 25 nm and 250 nm was built. First tests with the aerodynamic lens as aerosol inlet are currently in progress.

Markus Weber, Christoph Haisch

Funding
IWC-TUM

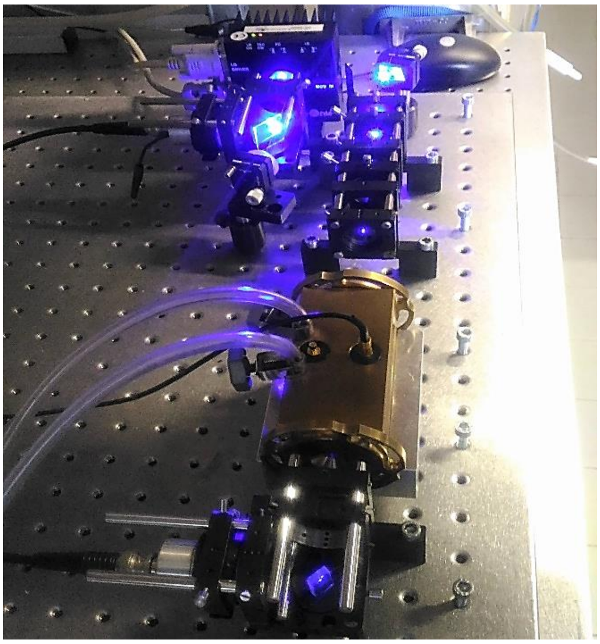
Fundamentals of Aerosol Photoacoustic Spectroscopy

Photoacoustic spectroscopy (PAS) is a technique based on the optical absorption of a modulated light beam by solids, liquids, or gases. The absorbed optical energy is converted into heat, leading to the expansion of the absorber and the surrounding medium. As the light is modulated, also this expansion is modulated, which in case of gas phase analysis means that a sound wave is formed. For particles smaller than the excitation wavelength, the intensity of this sound wave is generally assumed to be proportional to the total absorbing mass of the particles [1]. Our research is focused on the fundamental understanding of the PAS signal generation on particles.

State of the Art. PAS is currently routinely applied in aerosol characterization and exhaust gas analysis. Our study wants to exploit a combination of single particle, particle ensemble, and theoretical PA studies, addressing the two main issues in the field; i.e. the particle size dependence of the PA response and light absorption under high relative humidity conditions.

Analytical Approach. In collaboration with ETH Zurich (Laboratory for Physical Chemistry) two different systems have been employed: ensemble PAS (E-PAS) and single particle PAS (SP-PAS)[2]. E-PAS is more versatile and robust, allowing the analysis of a greater variety of particles, whereas the SP-PAS lets a very precise control of the specific particle, as for instance a high-precision size, chemical composition and homogeneity characterization (core/shell particles).

Results. Preliminary measurements have been performed under known controlled conditions using NO_2 in order to test and calibrate the system. First results have shown that the behaviour of the photoacoustic signal is closely related to the level of humidity, a crucial aspect for the study of aerosols in the atmosphere.



Experimental setup for ensemble photoacoustic spectroscopy: resonator cell 4kHz and Laser diode 445 nm.

Emilio Ambra

References

[1] C. Haisch, Measurement Science & Technology 2012, 23.

[2] J. W.Cremer, K. M. Thaler, C. Haisch, R. Signorell, Nature Communications 2016, 7(1)

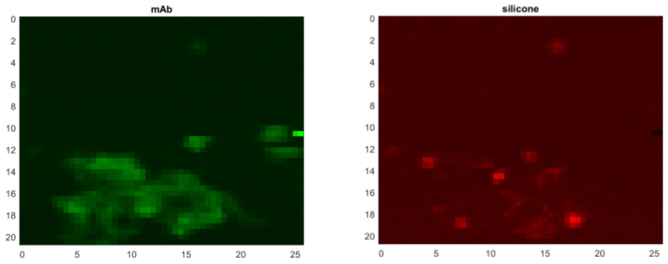
Funding
IWC TUM

Cooperation
ETH Zurich

Raman-based monitoring of protein aggregation

Formation of aggregates and particulates in biopharmaceutical formulation continues to be one of the major quality concerns in biotherapeutics development. State of the art Raman microscopes are able to analyze particulate matter in terms of number, size and shape based on microscopic images. The chemical composition of identified particles from 0.5 µm to 47 mm can be automatically determined via the generation of single Point Raman spectra and spectral correlation with a reference database. 3D-imaging of microscopically homogenous looking particles visualizes silicone majorities and identifies heterogeneous particles.

State of the Art. The formation of particles can be promoted by different mechanisms like unfolding of protein and adherence of hydrophobic regions or interaction of proteins with interfaces. Particles consist of different materials like protein, debris, and silicone oil. Micro-Flow Imaging techniques use microscopic images of particles for counting and sizing. Particle shape and size gives no information about the chemical identity [1].



Raman maps of protein aggregates: in green protein mass, in red silicon.

Analytical Approach. Raman microscopy can chemically distinguish between different materials such as protein and silicone. A solution containing 2 g/L monoclonal antibody was rigorously stirred for 30 seconds and analyzed by Raman microscopy. Silicone particles were generated by pumping Histidine buffer through silicone tubing. The suspension was analyzed by Raman Microscopy.

Results. Generated particles were analyzed with a WITec Raman alpha 300R using the 532 nm laser line. Large area scans (x/y axis) of particles were performed by acquiring Raman spectra from a point raster spaced 250 nm. Raman spectral maps were processed by spike removal and regressed with reference spectra of pure protein and silicone. Average spectra of the identified components were calculated and intensity distribution images of the components were generated. The figures represent protein in green and silicone in red.

Christian Haase

References

(1) Rygula et al., J. Raman Spectrosc. 2013, 44, 1061–1076.

Funding
IWC TUM

Cooperation
LMU Munich

Analysis of semi-volatile substances on aerosol nanoparticles from internal combustion engines.

The potential threat to human health from sub-micro-meter particles is given not only by the particles ability to deeply penetrate into the lungs, but also by their role as mean of transport for other possibly harmful substances.[1] For this reason, a setup based on the spectroscopy technology was developed, in order to have a real time detection of the target pollutants, mainly PAH, with a high time resolution.

State of the Art. In order to analyze the exhaust gases and get information about the particles composition, in most of the research the technique of the single particle analysis operating with Time of Flight mass spectrometers[2] or the collection on filtering media are currently exploited. In the first case, only the analysis of relatively big particles is possible, losing the information related to the small fraction (<50 nm), in the second one, a real time information during the sampling is not compatible with the method.

Analytical Approach. The system combines an IR-heating device (HELIOS), capable of desorbing substances from the aerosol surface, followed by a novel ionization source (SICRIT), and an ion trap mass spectrometer. Experiments under controlled conditions, with known substances of well-defined coating layer thickness serve for calibration. Further experiments in field measuring the end-of-pipe exhaust gases where conducted

Set up operating in a field campaign: sampling the exhaust gases from an old model motorbike.

Results. The results showed a coherent behaviour with an increasing signal corresponding to increasing concentrations of the substances. The results during the field campaign are coherent with the literature [3], showing a positive signal for the typical PAH expected after incomplete combustion.

Lorenza Gilardi, Klemens M. Thaler

References

(1) Donaldson, K., Stone, V., Clouter, A., Renwick, L., & MacNee, W., Occupational and Environmental Medicine. 2001, 58(3), 211-216.

(2) Lee A. K. Y.; Willis M.D.; Haely R. M.; Onasch T. B.; Abbatt J. P. D., Mixing state of carbonaceous aerosol in an urban environment: single particle characterization using the soot particle aerosol mass spectrometer (SP-AMS). Atmos. Chem. Phys. 2015, 15, 1823–1841.

(3) Erickson M. H.; Gueneron M.; Jobson B. T., Measuring long chain alkanes in diesel engine exhaust by thermal desorption PTR-MS. Atmos. Meas. Tech. 2014, 7, 225–239.

Funding

Bayerische Forschungsstiftung

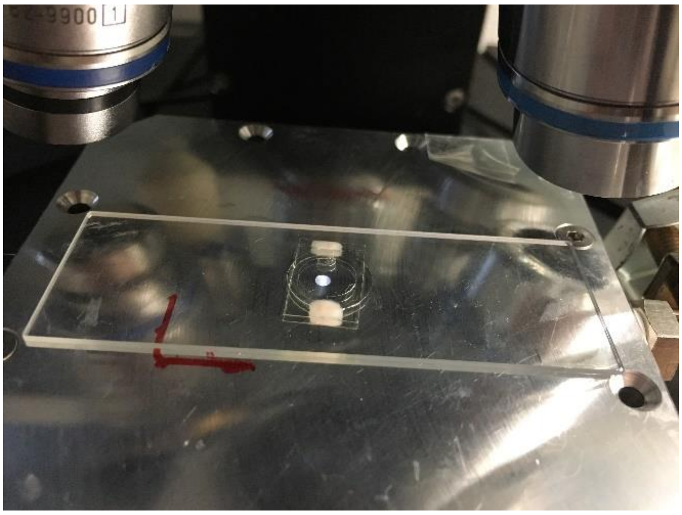
Cooperation

MAN Truck and Bus, Lehrstuhl für Verbrennungskraftmaschinen, Technische Universität München, Continental Emitec GmbH, Analytik Service Gesellschaft mbH

Raman mapping for the detection of living bacterium combing isotope method

Mycobacterial infections are difficult to treat threatening human health worldwide. Isotope method combing with Resonance Raman microscopy mapping provides us the information of specific substance distribution at single organism level, which help us to learn how mycobacteria grow.

State of the Art. *Mycobacteria smegmatis* has been investigated for mycobacterial physiology as a model because of its fast-growing and nonpathogenic in lab. Raman mapping combining with isotope can provide shift vibrational information on the level of single organism. It is helpful for us to learn some diseases.



M.semgmatis cells fixed and put on a temperature controller

Analytical Approach. Firstly, mycobacteria cells cultivated overnight and fixed on hydrophobic glass slides observing their regrowth under microscopy to find out the best growing parameters (such as temperature). Then, bacteria regrowth is observed in D_2O medium to find out the best content that does not influence bacteria growth.

Finally, Raman microscopy was used for data collection at different time points at single organism level during the growth. The results evaluated with MATLAB.

Results. We have found the proper condition for *M. smegmatis* regrowth in a measurement cell, and obviously seen new Raman peaks split when addition D_2O labeled medium for bacteria regrowth. However, the Raman data mapping for substances distribution in single organism is not that clear. Further optimization of the experimental conditions will be performed.

Li Qiu, David Bauer

References

(1) Saviola B., Pigments and Pathogenesis. J. Mycobac. Dis. 2014, 4:5

(2) Roberta P., Dana K., Valentina D., Daniel E., Mamadou D., , Gilles E., Riccardo M., Jean-Marc R., SigF Controls Carotenoid Pigment Production and Affects Transformation Efficiency and Hydrogen Peroxide Sensitivity in Mycobacterium smegmatis. J. Bacteriol. 2008, 7859-7863

Funding

TUM-IWC

China Scholarship Council

Cooperation

Max von Pettenkofer
Institute LMU

Kerosene from algae: chemical analysis of the cultivation medium

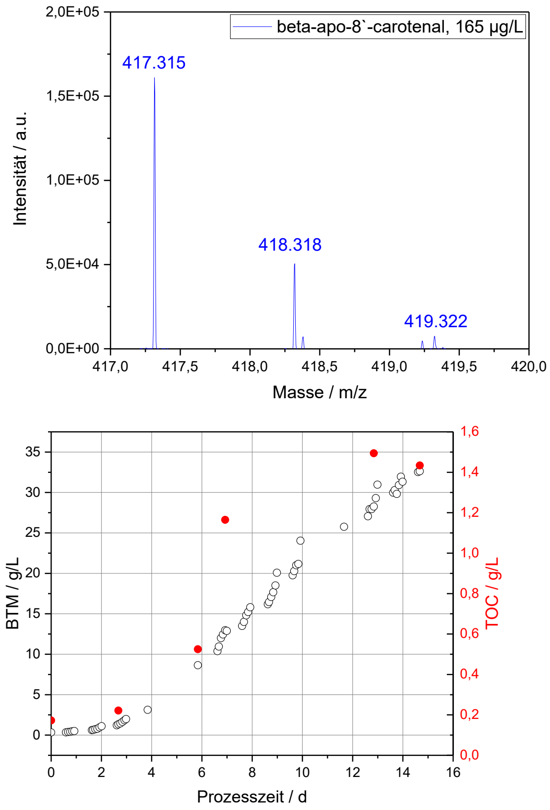
Air traffic volume is predicted to increase at an annual rate of more than 5 %, leading to a significant increase of kerosene consumption and CO_2 emission. The use of biogenic fuel can help archiving emission reduction. The partners in the project select and optimize microalgae in order to maximize the production of lipids, which are harvested and used to generate kerosene. This approach is highly promising, as it does not consume valuable clean water and agricultural area. Recirculation of the salty water further reduces consumption of raw material. However, it has to be made sure that during this recirculation, no algae toxins or other secondary metabolites hampering the cultivation, are produced.

State of the Art. In the framework of the project “alpine algae kerosene”, algae are used to produce green kerosene. During the process of algae cultivation, secondary metabolites and bacteria can be accumulated in the cultivation medium, thus hindering algae growth and can lead to contamination of wastewater. We support our cooperation partners by continuously monitoring critical compounds of the growth medium analytically.

Analytical Approach. As carotenes and chlorophyll and there metabolites are suspected to influence the algae growth, we developed an APCI-MS method for these two compounds. The ion content of the growth medium is now monitored continuously throughout the cultivation by ion chromatography. Additionally, we started to monitor total and dissolved organic content (TOC and DOC).

Results. A limited supply of various ions was identified as a limiting factor of algae growth. Currently, we try to verify the hypothesis that also carotenes are also influencing the cultivation, either biochemically or due to their optical absorption properties, which limit the light penetration into the medium, which is essential for algae growth.

Dr. Anna Neumann, Katharina Zirrngibl, Dr. Klemens Thaler



MS spectra of beta-carotene (top) and temporal behavior of the TOC in the growth medium.

Funding

Bayerisches Staatsministerium für Wirtschaft und Medien, Energie und Technologie

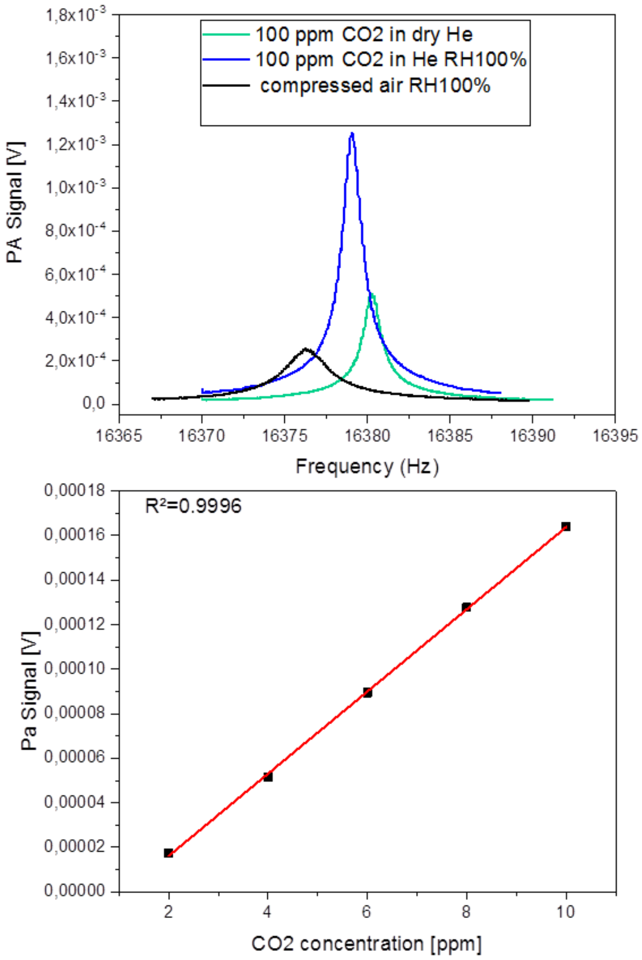
Cooperation

Werner Siemens-Lehrstuhl für Synthetische Biotechnologie, Lehrstuhl für Bioverfahrenstechnik, Lehrstuhl für Bioverfahrenstechnik, all TU München, Bauhaus Luftfahrt e. V.

Development of a photoacoustic-based δ^{13}C Detector

Abstract: Compound specific carbon isotope analysis (CSIA) provides additional and often unique means to (i) allocate sources, and (ii) identify degradation processes of micropollutants in water. The most common technique for isotope analysis is the isotope ratio mass spectrometry (IRMS) that allows an impressive level of precision, typically near 0.1‰. However, IRMS has shortcomings.

State of the Art. The goal of this work is combining the quartz-enhanced photoacoustic (QEPAS) technique with the excellent benefits of Quantum Cascade Laser (QCL) source to develop a GC-coupled stable carbon isotope detector. The QEPAS detector use quartz tuning fork as sharply resonant acoustic transducer to measure the CO_2 concentration. In comparison to the IRMS, it is compact, robust, portable, easy to operate (even under field condition), free from isobaric interferences and isotope effects that can be coupled to the GC without open split, reduction and drying unit.



a) Resonance curves of CO_2 in different gas matrices
b) CO_2 calibration curve in wet helium (RH100%)

Analytical Approach. In order to be competitive with IRMS, the QEPAS system must reach a CO_2 sensitivity level of 100 ppb and a sampling rate of 20 Hz.

Results. Based on the first measurement results, the signal strength strongly depends on the gas matrix (Fig. a). Due to the slow V-T relaxation of CO_2 in He and in air with respect to the modulation frequency, the thermal waves in the gas cannot follow fast changes of the laser induced molecular vibration excitation. Because the H_2O molecules promote the V-T relaxation, in saturated sample gas a promising sensitivity level of 160 ppb can be reached based on the calibration results (Fig. b). However, the disadvantage of the excellent resonant properties is an increased response time, which does not allow to reach the required sampling rate. The new prototype is equipped with a microresonator, which ensures not only a greater sensitivity, but a shorter response time.

Noemi Utry, Klemens M. Thaler, Christoph Haisch

Funding
IWC TUM

References

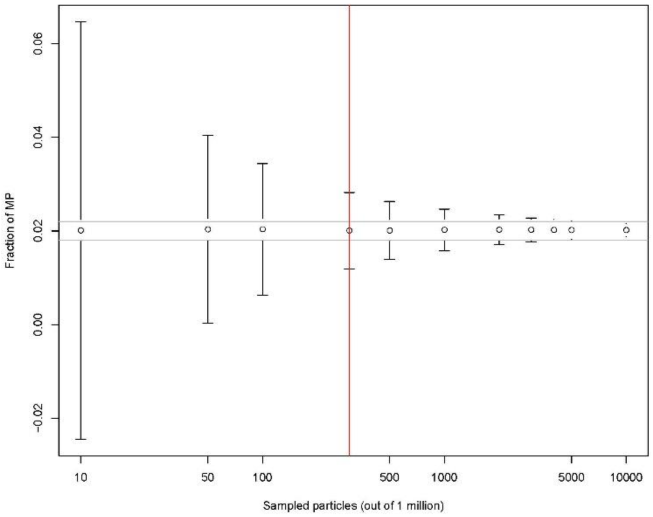
(1) Kosterev, A.A.; Bakhirkin Y.A.; Curl R.F.; Tittel F.K. (2002) Quartz-enhanced photoacoustic spectroscopy. Opt. Lett., 27, 1902–1904.

Microplastic particle analysis from a statistical point of view

Currently, microplastic (MP) particle analysis by means of Raman microspectroscopy (RM) is a cumbersome process. An average filter sample is covered with up to millions of individual particles. Analyzing every one of them requires weeks or even years of measurement time. We applied a simple statistical tool to estimate the minimal number of particles that need to be analyzed for a statistically sound result.

State of the Art. MP (<5 mm), is an environmental problem of public concern. Its toxicity is a field of debate and yet not fully understood.[1] Nevertheless, the particulate nature makes MP an interesting analyte. One of the numerous challenges to face is the analysis of the filter sample by means of RM. In this regard up to millions of particles can cover a filter. Measuring all of them could take several days or even up to years, depending on the used acquisition time.

Analytical Approach. The problem of particles on a filter was simplified by postulating an ideal measurement system, normal particle distribution and categorizing the particles into MP and non-MP.[2] The statistical approach is called simple random sample of units selected without replacement (*srswor*). The overall number of particles, the estimate of the MP fraction and an allowed margin of error are used to calculate a number of particles that need to be measured to yield a statistically sound result by analyzing a representative fraction of the particles.



Correlation of sample size and margin of error *e* for a 2% MP fraction; grey line - margin of error *e* = 10%; red line – typical sample size of 300 particles

Results. In the figure an exemplary calculation is displayed. We assumed one million particles on the filter sample. The estimated MP fraction is 2% and the allowed margin of error is 10%. For this case it would be sufficient to analyze 13 000 particles to determine the 2% ± 0.2% MP particles.

Philipp M. Anger and Elisabeth von der Esch

References

(1) Triebskorn, R.; Braunbeck, T.; Grummt, T.; Hanslik, L.; Huppertsberg, S.; Jekel, M.; Knepper, T. P.; Krais, S.; Müller, Y. K.; Pittroff, M.; Ruhl, A. S.; Schmieg, H.; Schür, C.; Strobel, C.; Wagner, M.; Zumbülte, N.; Köhler, H.-R., Relevance of nano- and microplastics for freshwater ecosystems: A critical review, Trends Anal. Chem. 2019, 110, 375-392.

(2) Anger, P. M.; von der Esch E.*; Baumann, T.; Elsner, M.; Niessner, R.; Ivleva, N. P., Raman microspectroscopy as a tool for microplastic particle analysis, Trends Anal. Chem. 2018, 109, 214-226. (* shared first authorship)*

Funding

Bundesministerium für Bildung und Forschung

Bayerische Forschungsstiftung

IWC-TUM

Cooperation

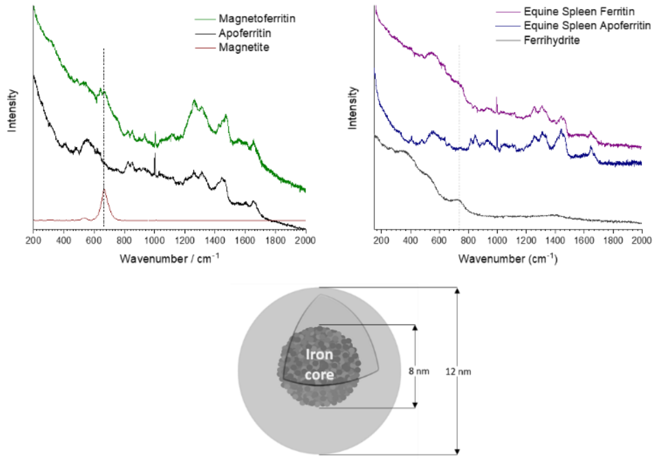
Mikroplastik im Wasserkreislauf (MiWa)

Mikropartikel in der aquatischen Umwelt und in Lebensmitteln (MiPAq)

Raman analysis of bio-based magnetic nanoparticles

Ferritin is an iron-containing protein which has gained great interest because of its ability to biomineralize nano-sized particles. Such bio-based nanoparticles would open new opportunities in various applications in biological and medical fields.

State of the Art. Ferritin holds potential of a bio-based nanoparticle since this protein is a globular shaped protein with an iron core of about 8 nm located inside its cavity. Being bio-based, ferritin may have various advantages regarding the toxicity and biocompatibility especially as a source magnetic nanoparticles. However, to improve the magnetic properties, attempts to modify natural ferritin into magnetoferritin have already been established.[1]



Top: left: Raman spectrum of magnetoferritin, apoferritin and magnetite reference; right: Raman spectrum of natural ferritin, apoferritin and ferrihydrite reference.
Bottom: Schematic illustration of ferritin.

Analytical Approach. For a better understanding of the molecular processes of biomineralization mechanisms of the iron core in ferritin and magnetoferritin, Raman spectroscopy has been proved to be a suitable tool for an on-time analysis. This method provides spectra which are unique to each compound and structure with a spatial resolution in µm-range. Therefore, it is possible to distinguish between various iron oxides and hydroxides, even if they are incorporated in the protein and despite of the complexity of the Raman signature of proteins.

Results. In Raman spectra of ferritin and magnetoferritin we observe the anticipated bands of proteins and an additional broad band indicating the presence of iron compounds. As expected, this band cannot be seen in the Raman spectrum of apoferritin, which is the protein without the iron core. Differences in the Raman spectra of ferritin and magnetoferritin can be seen, revealing that the iron core of natural ferritin is composed of ferrihydrite[2] and of magnetoferritin is made of magnetite[1].

Carolin Hartmann

References

(1) Massner, C., Sigmund, F., Pettinger, S., Seeger, M., Hartmann, C., Ivleva, N. P., Niessner, R., Fuchs, H., Hrabě de Angelis, M., Stelzl, A., Koonakampully, N. L., Rolbiesky, H., Wiedwald, U., Spasova, M., Wurst, W., Ntziachristos, V., Winklhofer, M., Westmeyer, G. G. Genetically Controlled Lyosomal Entrapment of Superparamagnetic Ferritin for Multimodal and Multiscale Imaging and Actuation with low Tissue Attenuation. Adv. Funct. Mater. 2018, 28, 1706793.

(2) C. Hartmann, M. Elsner, R. Niessner, N. P. Ivleva, Nondestructive Chemical Analysis of the Iron-Containing Protein Ferritin Using Raman Microspectroscopy. Appl. Spectrosc. 2019 doi.org/10.1177/0003702818823203.

Funding

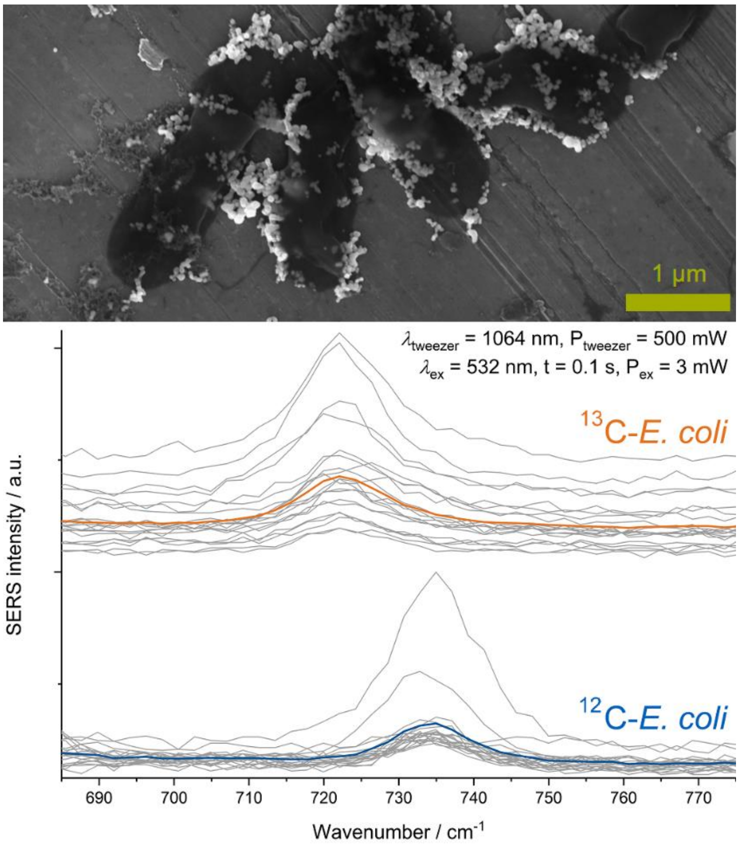
Deutsche Forschungsgemeinschaft (DFG), International Graduate School of Science and Engineering (IGSSE).

Cooperation

Prof. Dr. G. G. Westmeyer, Institute of biological Imaging, IBMI, TUM.

Stable isotope Raman microspectroscopy and SERS for analysis of microorganisms on the single-cell level

Microorganisms play an essential role in most ecosystems and in human health. Therefore, it is crucial to develop reliable and sensitive methods for the detection, discrimination and analysis of their activity. Raman microspectroscopy in combination with a stable isotope approach is an emerging tool for the nondestructive characterization of the molecular and isotopic composition of microorganisms on the single-cell level.



Scanning electron microscopy of *E. coli* with Ag nanoparticles (top); consecutive SERS spectra of optically trapped and unlabeled or ^{13}C-lablled *E. coli* cells (bottom).

State of the Art. Stable isotope Raman microspectroscopy (SIRM) provides characteristic fingerprint spectra of samples with the spatial resolution in the µm-range, containing information i) on stable isotope-labeled substances and the amount of a label and ii) on the chemical composition and structure of samples.

Analytical Approach. SIRM allows *in situ* investigations of ecophysiology and metabolic functions of microbial communities without interference of water. Furthermore, the sensitivity of RM and SIRM analysis can be significantly improved (in the range of $10^3 – 10^6$) due to surface-enhanced Raman scattering (SERS), e.g. by using of Ag nanoparticles. In contrast to RM and SIRM (where whole-organism fingerprints for bacteria are obtained), SERS provides information on substances at the surface of cells.

Results. Analysis of the model bacterium *E. coli* revealed that the SERS intensity and the number of hits depend on different factors (storage time, presence of D_2O) and reflects the metabolic activity of cells. By employing optical trapping, we were able to distinguish between unlabeled and stable isotope-labeled cells in fluids. Our findings can open new possibilities for the application of SIRM and SERS to probe for the activity of microorganisms on the single-cell level.

Ruben Weiss and Natalia P. Ivleva

Reference

Weiss, R.; Palatinszky, M.; Wagner, M.; Niessner, R.; Elsner, M.; Seidel, M.; Ivleva, N.P. Surface-enhanced Raman spectroscopy of microorganisms: limitations and applicability on the single-cell level. Analyst 2019, 144, 943-953

Funding

Deutsche Forschungsgemeinschaft, DFG (IV 110/2-1)

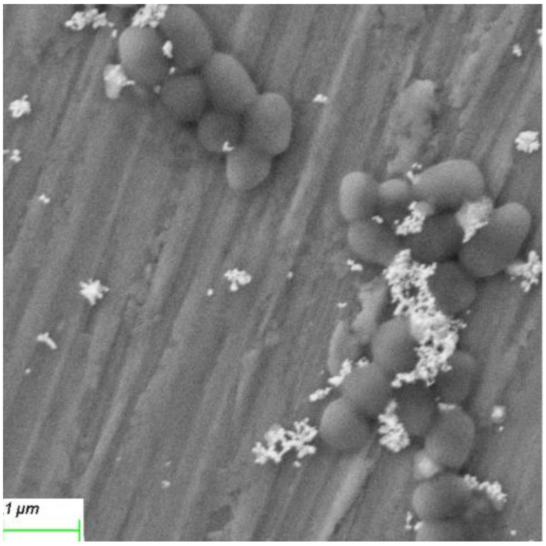
Cooperation

Prof. Dr. Michael Wagner, University of Vienna, Division of Microbial Ecology, Austria

Bioorthogonal noncanonical amino acid tagging–surface enhanced Raman scattering (BONCAT-SERS) for visualization of active bacterial cells

Determination of active bacterial cells responsible for micropollutant degradation can increase efficiency of the water treatment. Combination of BONCAT and SERS can visualize and characterize active cells. Since active cells incorporate tagged amino acids (TAAs) the modified nanoparticles (NPs) can be attached to the surface via click chemistry reaction. So, bound Ag NPs enhance Raman signal of the active cells.

State of the Art. Removal of organic pollutants in water is crucial for drinking water quality and for aqueous ecosystems. Identification and characterization of microorganisms responsible for degrading organic pollutants is challenging and important for ensuring the sustained and cost efficiency water treatment. Most current methods do not disclose who is really metabolically active and growing, are expensive and/or may disturb the studied systems or reveal active cells in time-consuming and cost-intense mode with restriction to explore only cultured microorganisms. So, a minimally invasive, rapid, and sensitive approach that combines visualization and characterization of active cells is warranted.



SEM image of pollutant degrader *Arthrobacter aurescens* TC1 with AgNP

Analytical Approach. The proposed approach pillars on a combination of BONCAT with SERS. BONCAT relies on the *in vivo* incorporation of amino acids surrogates into bacterial biomass and is used to study individual cell response to external signals *in situ*. SERS is based on Raman spectroscopy and uses metal (Au or Ag) NPs to enhance the Raman signal.

Results. With fluorescence microscopy we determined incorporation of TAAs by the atrazine degrader *Arthrobacter aurescens* TC1. Raman microspectroscopy and SERS with silver NPs revealed no changes in bacterial cells incorporating TAAs in polluted media compared to the control cells. Scanning electron microscopy (SEM) showed integrity of bacterial cells and distribution of NPs on their surface. Alkyne-modified silver NPs were synthesized according to Shi et al.

Oleksii Morgaienko

References

1) Hatzenpichler, R.; Connon, S. A.; Goudeau, D.; Malmstrom, R. R.; Woyke, T.; Orphan V. J., Visualizing in situ translational activity for identifying and sorting slow-growing archaeal−bacterial consortia. PNAS, 2016, 113, (28), 4069-4078.

(2) Shi, L.; Jing, C.; Ma, W.; Li, D.-W.; Halls, J. E.; Marken F.; Long, Y.-T., Plasmon Resonance Scattering Spectroscopy at the Single-Nanoparticle Level: Real-Time Monitoring of a Click Reaction. Angew. Chem. 2013, 125, (23), 6127-6130.

Funding
IWC-TUM

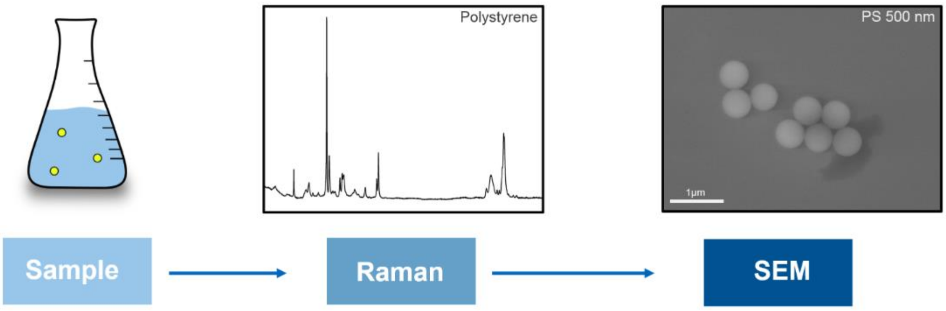
Cooperation
Dr. T. Lueders, Dr. S. Marozava (Helmholtz-Zentrum München)

Raman microspectroscopy for the analysis of submicrometer plastic particles

The analysis of environmental plastic particles in the submicrometer range poses a challenge for the established techniques. We develop a method that combines Raman microspectroscopy and scanning electron microscopy for chemical and morphological characterization of small environmental plastic particles.

State of the Art. Plastic waste persists in the environment, where it breaks down to increasingly small particles, called microplastic (MP, 1 µm – 5 mm), subµ-plastic (0.1 µm – 1 µm) and nanoplastic (1 nm – 100 nm). Subµ- and nanoplastic have been shown to behave differently than MP. However, methods for the analysis of subµ- and nanoplastic are still scarce and the current protocols only provide chemical information on the collected plastic material of the sample, i.e. bulk analysis. In many instances, it is, however, important to perform a single particle analysis.

Analytical Approach. Raman microspectroscopy (RM) allows the chemical identification of environmental plastic particles down to 0.25 µm, which is the diffraction limit for typical RM setups. We combine RM with scanning electron microscopy (SEM) to provide both the spectroscopic information and high resolution imaging (see figure).



The coupling of RM and SEM provides optical and electron microscopic images as well as a chemical Raman map.

Results. Coupling of RM and SEM has been tested with synthetic subµ-polystyrene beads with sizes of 500 nm and even below. For this, an appropriate sample substrate had to be found. This combination of methods gives the chemical (RM) and visual (SEM) information on the polystyrene subµ-particles, highlighting the high resolution of the SEM that gives a morphological characterization and a spectroscopic analysis of the individual particles. Furthermore, artificially fragmented subµ-plastic particles, made from polystyrene, have been used to demonstrate the applicability of this method for environmentally relevant particles.

Christian Schwaferts

Reference

Schwaferts, C., R. Niessner, Elsner, M., Ivleva, N. P., Methods for the analysis of submicrometer- and nanoplastic particles in the environment. Trends Anal. Chem. 2019, 112, 52-65

Funding
BMBF SubµTrack

Cooperation
Prof. Dr. Drewes, Chair of Urban Water Systems Engineering, TUM;
Postnova Analytics GmbH;
BS-Partikel GmbH

Microplastic particle analysis from an automation point of view

A statistically sound analysis of microplastic requires the measurement of thousands of individual particles from each sample. Therefore, automation is key to enable such an analysis in a reasonable amount of time.

State of the Art. Microplastic (MP) particles (plastic fragments 1 µm – 5 mm) can already be characterized through automated Raman microspectroscopy (RM).[1] An important step for the automated Raman measurement is the detection of particles and calculation of measurement points, which needs to be further refined.

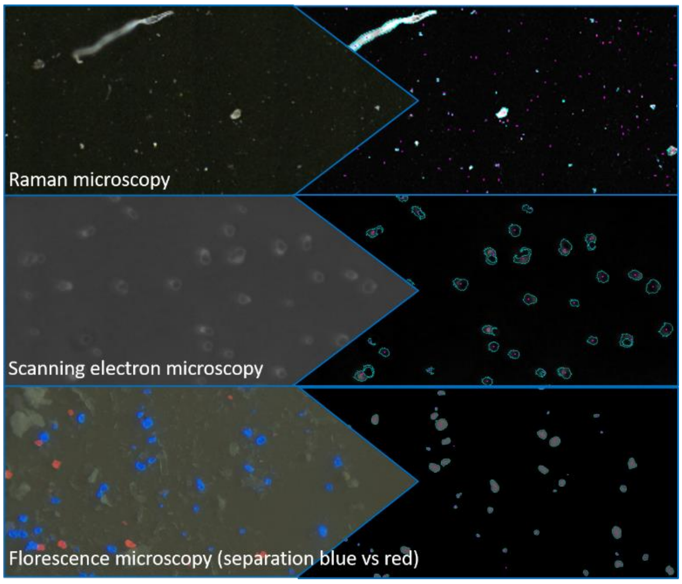


Image based particle detection and morphological characterization for varying instrumentation.

Analytical Approach. A MP sample is collected on a filter, making all deposited particles interesting targets for measurement. Before the targets can be chosen, ideally, all particles need to be localized via image processing. To achieve this goal, filter material and planarity, as well as image capture and processing were optimized. Furthermore, the detection program was expanded to cater to the needs of our *SubµTrack* and *MiPAq* partners, by including the analysis of MP particles in SEM and fluorescence microscopy images.

Results. So far, it is possible to detect particles, spheres and fibers as small as 10 µm on a filter surface of 16000 µm^2 (20× magnification) with RM. These particles can be morphologically analyzed, and coordinates can be calculated that ensure a measurement within the selected particle. Currently these coordinates are imported into our RM system for automatic measurement. Future versions of the program will allow: i) the analysis of particles <10 µm, ii) the option of direct control of the RM as well as iii) export of coordinate lists to keep it applicable for all RM systems, SEM and fluorescence microscopy. Furthermore, the number of randomly selected particles will be automatically calculated (*srswor*) and measured.

Elisabeth von der Esch, Philipp M. Anger, Leonard Prechtl and Alexander J. Kohles

Reference

(1) P. M. Anger, E. von der Esch*, T. Baumann, M. Elsner, R. Niessner, N. P. Ivleva, microspectroscopy as a tool for microplastic particle analysis, Trends Anal. Chem. 2018, 109, 214-226.Trends Anal. Chem.* ***2018****, 109, 214-226. (* shared first authorship)*

Funding

Bayerische Forschungsstiftung

Bundesministerium für Bildung und Forschung

IWC-TUM

Cooperation

Mikropartikel in der aquatischen Umwelt und in Lebensmitteln (MiPAq)

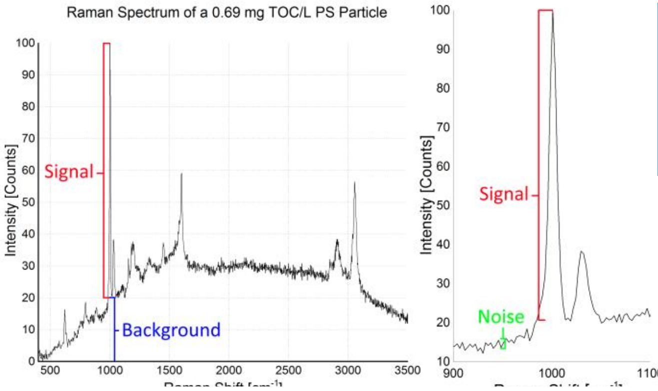
Mikroplastik im Wasserkreislauf (MiWa)

Microplastic particle analysis from an interference interaction point of view

Environmental microplastic can be found in various matrices and is very rarely present in its pristine form. By studying the interaction of humic substances with microplastic particles, the limitations for their detection by Raman microspectroscopy can be estimated.

State of the Art. So far it is widely accepted that fluorescence of environmental samples is a problem for the analysis with Raman microspectroscopy.[1,2] But it is unclear if the interaction of microplastic (MP) with fluorescence inducing compounds, e.g., humic substances inhibits their detection.

Analytical Approach. To assess if humic substances inhibit the detection of microplastics (MP) three different polymers (polylactic acid (PLA), polystyrene (PS) and polypropylene (PP)) were fragmented and exposed to different humic substance concentrations in water. These polymers were chosen as they represent polymers with heteroatoms in the backbone, polymers with aromatic groups and pure hydrocarbons. The resulting fragments were filtrated and measured by automated Raman microspectroscopy. From the collected spectra a signal to background and signal to noise ratio was determined to evaluate the detectability of the polymer fragments.



Determination of signal to background and signal to noise ratio to estimate detectability of MP.

Results. From these ongoing investigations it is apparent that the interaction of humic substances with MP is polymer specific and, therefore, leads to varying degrees of fluorescence background. For all polymers the signal to background ratio decreases with rising humic acid concentrations, making the MP harder to detect. In the case of PP fragments below 30 µm were undetectable at 0.69 mg TOC/L from humic substances and a concentration of 3.45 mg TOC/L rendered particles of all sizes undetectable. On the contrary PS was always detectable even to sizes below 10 µm. With these findings we show that for most samples taken from lakes and rivers (total organic carbon TOC << 3.45 mg/L) the detection of MP is possible without removal of organic matrices as the fluorescence interference does not prevent the detection of most polymers. If the TOC rises above this level it is advisable to employ organic removal steps before analysis.

Elisabeth von der Esch and Merlin Junk

References

(1) *Anger, P. M.*; von der Esch, E.*; Baumann, T.; Elsner, M.; Niessner, R.; Ivleva N P, Raman microspectroscopy as a tool for microplastic particle analysis, Trends Anal. Chem. 2018, 109, 214-226.* (shared first authorshiop) *(2) Ivleva, N. P.; Wiesheu, A. C.; Niessner, R., Mikroplastik in aquatischen Ökosystemen, Angew. Chem. Int. Ed. 2017, 129, 1744-1764.*

Funding

Bayerische Forschungsstiftung

IWC-TUM

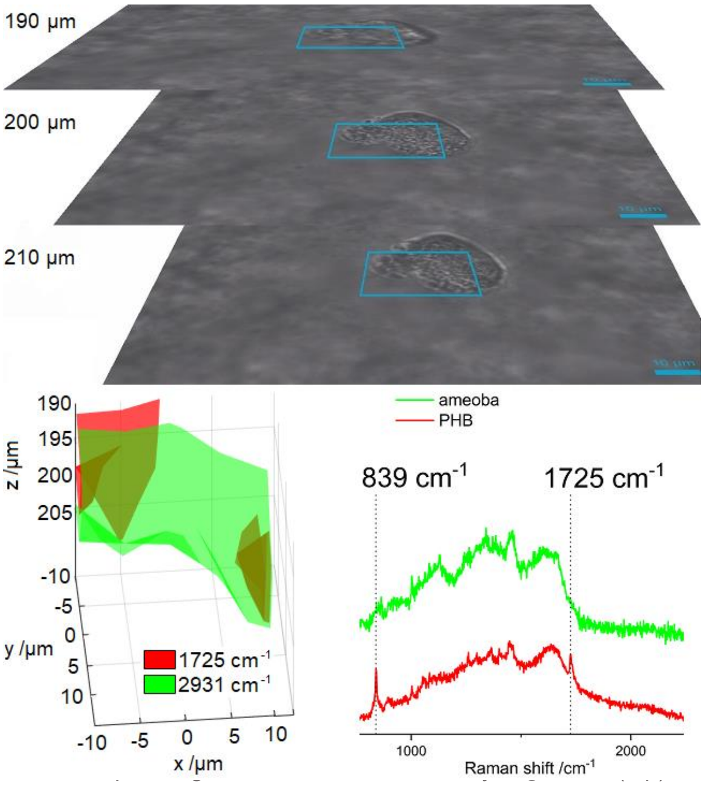
Cooperation

Mikropartikel in der aquatischen Umwelt und in Lebensmitteln (MiPAq)
`

3D Raman microspectroscopy of microbial samples

Microorganisms play a major role for degradation and fate of pollutants. Some microbes directly affect the health of humans. The three-dimensional analysis of microbial samples by Raman microspectroscopy (RM) enables the spatially resolved detection of microorganisms and a better understanding of biofilm-related processes.

State of the Art. Microbial life appears in complex communities predominantly structured in biofilms.[1] The occurrence of pathogens in biofilms may hamper disinfection methods but also increase their virulence as for the case of *Legionella*.[2] Common techniques for the discrimination of microorganisms include cultivation, genome sequencing, fluorescence staining and immunoassays.



iso-surface plot of Raman signals in the blue highlighted volume (bottom left); corresponding Raman spectra of amoeba and polyhydroxybutyrate: PHB (bottom right).

Analytical Approach. The Raman spectroscopic approach needs only minimal sample preparation and combines several advantages. It is non-invasive, three-dimensionally resolved, shows little interference of water and offers chemical information, even the incorporation of stable isotopes. Ideally, the spatial resolution in the micrometer range is sufficient to locate bacteria inside of larger microorganisms such as amoeba and thus, potentially evading false-negative results of other detection methods.

Results. The 3D RM analysis of environmental samples contaminated with *Legionella* illustrates the capabilities of this analytical technique for the study of biofilms. The spectroscopic and spatial information available by RM may enhance the insights into this ecosystem.

Ruben Weiss, Michael Seidel and Natalia P. Ivleva

References

(1) Widder, S.; Allen, R.J.; Pfeiffer, T.; Curtis, T.P.; Wiuf, C.; Sloan, W.T.; Cordero, O.X.; Brown, S.P.; Momeni, B.; Shou, W.; Kettle, H.; Flint, H.J.; Haas, A.F.; Laroche, B.; Kreft, J.-U.; Rainey, P.B.; Freilich, S.; Schuster, S.; Milferstedt, K.; van der Meer, J.R.; Großkopf, T.; Huisman, J.; Free, A.; Picioreanu, C.; Quince, C.; Klapper, I.; Labarthe, S.; Smets, B.F.; Wang, H., Challenges in microbial ecology: building predictive understanding of community function and dynamics. ISME J. 2016, 10, 2557-2565.

(2) Scheikel, U.; Tsao, H.-F.; Horn, M.; Indra, A.; Walochnik, J., Free-living amoebae and their associated bacteria in Austrian cooling towers: a 1-year routine screening. Parasitol. Res. 2016, 115, 3365-3374.

Funding

Federal Ministry of Education and Research (BMBF project 13N13698: LegioTyper)

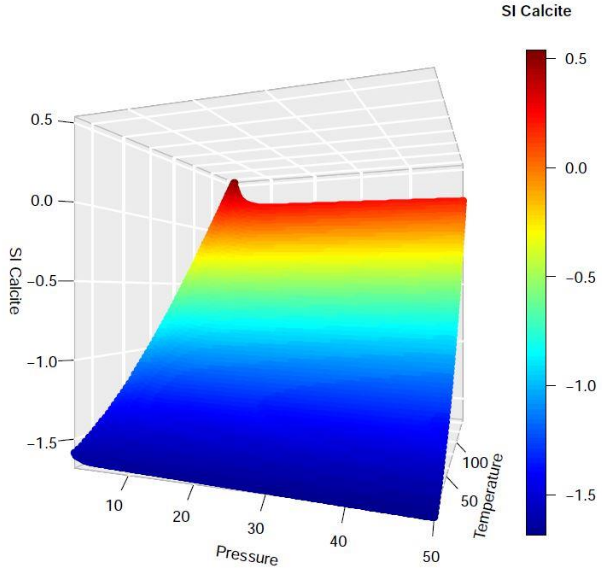
Flexibility options for geothermal power generation

Hydrogeochemistry and reservoir conditions allow more flexibility than the power plant and the pumps. Future geothermal power plants might contribute to a volatile energy market.

The problem of volatile renewable energy sources. Finally, renewable energy sources are contributing significantly to the national energy market. Although weather conditions and energy became much more predictable of the years, there is still a need for short term control reserves to cover a sudden energy demand or overproduction. This project focussed on the potential of geothermal power plants to provide a control reserve.

Hydrochemical aspects. The effects of quickly changing flow rates and temperatures on a stable operation of the power plants, at the pumps and in the reservoir are assessed using hydrogeochemical models. The simulations were run for typical sites in the Bavarian Molasse Basin (BMB), the Upper Rhine Valley (URV) and the North German Basin (NGB). Recorded real time operation data was used as input for a dynamic hydrogeochemical model.

Results. Gradients recorded in operation data sets of the power plants in the BMB are much higher than the initial guesses, and geothermal plants providing district heating have always been run controlled by sometimes rapidly changing weather conditions. However, the inertia of the thermal water system limits the flexible operation to tertiary control reserve. The long-term operational data suggest a generally benign behaviour with just one exception: a complete shutdown and restart of the pumps has proven to increase the risk of failure and enhanced precipitations in and above the pumps. A simulation comparing the current operation and a hypothetical operation providing tertiary reserve by a variation of the flow rate and temperature spread showed no significant changes in terms of precipitates and dissolution rates in the reservoir.



Saturation index for calcite as a function of pressure and temperature for a site in the MB

Unfortunately, these positive results cannot be transferred to URV and NGB. In both regions the hydrochemical conditions favor precipitates at lower temperatures, therefore the injection wells are less fault tolerant and will react sensitively to temperature changes.

A flexible operation of the geothermal system makes sense with regard to a sustainable exploration of the reservoir, under the current subsidies for geothermal power, it makes more sense to run the power plant at full throttle; at least from a financial point of view.

T. Baumann

Funding

German Environment Agency
FKZ 37EV 16 114 0

Cooperation

TUM Institute for Energy Systems, TUM Chair of Renewable and Sustainable Energy Systems, TUM Chair of Hydrogeology, TUM Centre for Energy Markets, Bayreuth University LTTT

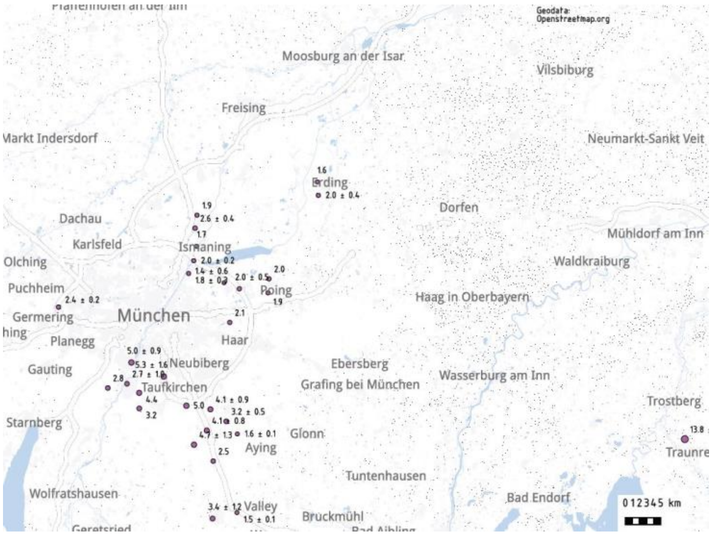
Hydrogeochemical Characterization of Geothermal Reservoirs

Reservoir characterization is the key to efficient heat mining and reservoir management, and hydrogeochemistry is fundamental to reservoir characterization.

Deep hydrogeothermal energy exploration in Bavaria is a continuous success story, even though during the past year a small number of very ambitious projects did not meet the expectations. On the other hand few seismic events, attributed to single projects, received large public interest and finally led to a public vote against a deep hydrogeothermal project in one small village close to Munich. These adverse developments underline the need for an accurate prediction of the reservoir behaviour.

Deviations of hydraulic, hydrochemical and temperature data from the predictions indicate, that although many of the processes in the reservoir are unterstood the parametrization of the reservoir might not be accurate enough for long term prediction. An interdisciplinary approach, connecting geology, hydrogeology, geophysics, geohydraulics, and hydrogeochemistry is required to improve reservoir management and efficiency of heat mining.

Results: The hydrogeochemical model of the Upper Jurassic nowadays allows a prediction of the hydrochemical conditions (cations, anions and gas phase) with significantly reduced uncertainty. Together with lithostratigraphic and structural data, this facilitates the design of multi-well facilities. The calibrated numerical models indicate that the dissolution rates at the injection wells are higher if water from a limestone reservoir is injected into a dolomite reservoir, compared to an injection vice versa or settings with homogeneous lithology. This further justifies the current design approach to produce from fractures and faults and to inject into the matrix.



Calcium-magnesium-ratio in the central molasse basin

Current work focusses on the parametrization of a model to quantify and predict the effects of the hydrogeochemical reactions on the hydraulics and mechanics of the boreholes and reservoirs. Another issue in this context is the assessment of precipitation of carbonates as the temperature of injected reservoir fluid is increasing. The latter, however, is not easily accessible through hydraulic data. Monitoring and reservoir management require more and continuous data. In order to reduce costs, multivariate and virtual sensors are required. Here, the framework Geothermie-Allianz Bayern can serve as a platform to aggregate data and to develop evaluation methods.

T. Baumann

Funding

BayStMWK (Geothermie-Allianz Bayern)

Cooperation

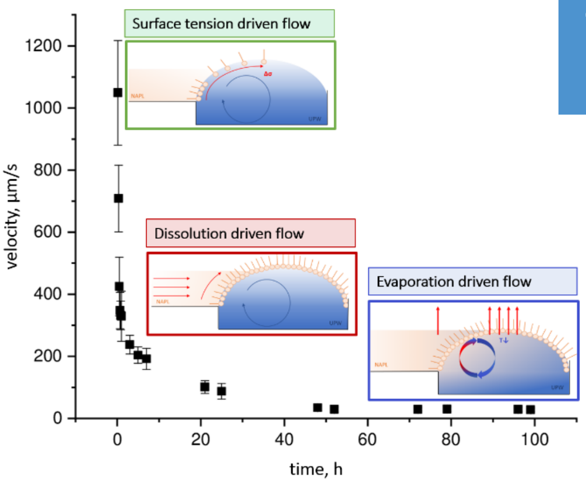
TUM Chair of Hydrogeology

Mass Transfer at Interfaces to Nonaqueous Phases

Abstract: In a combined experimental and numerical study, we aimed at verifying the theoretical basis of a fast-rotating, spontaneous quasi-stationary roll cell at a 1-octanol/water interface that sustains up to 99h. Through the parameterization of this flow phenomenon we experimentally decoded the overall process and quantified the impact of numerous physicochemical substance properties.

State of the Art. Interfacial processes are relevant for a broad range of natural and engineered processes. Local inhomogeneities at interfaces between immiscible phases are associated with interfacial instabilities that induce compensating currents and dissipative structures leading to an increased mass transfer as it significantly contributes to the mixing of the phases. These interfacial currents have been subject to considerable research, especially concentrating on interfacial instabilities leading to Marangoni convection that is induced by external interface tension gradients but also by spontaneous and local instabilities in temperature and concentration.

Analytical Approach. The objective of this study was to characterize and quantify the dynamics of a persistent movement in the form of a quasi-stationary roll cell along interfaces between water and NAPL by the conception of microfluidic models and quantitative parameterization. The convective flow was visualized with fluorescent particle tracers and an epifluorescence microscope with high temporal and spatial resolution. The velocities of the convective flow were measured experimentally by using single particle tracking. To quantify the impact of numerous parameters like physicochemical substance properties on the velocity of the interfacial convection several micromodels were developed. These tailored micromodels enabled the quantitative parametrization of the dominating driving forces of the long-lasting roll cell. The results of numerous test series provide a reliable data base for validating a numerical model that estimates the particle velocity as a function of liquid properties.



Time dependency of the velocity of the convective roll cell at a 1-octanol/water interface and the dominating mechanisms

Results. Based on the kinetics of the long-term experiment up to 9 h we postulate three acting mechanisms with different velocity rates and durations: (1) a fast decaying and short-lived surface tension driven flow that dominates the early stage (Marangoni convection), (2) a sustaining but decaying medium-lived dissolution driven flow and (3) a long-lived evaporation driven flow that sustains the fluid motion. It was experimentally found that these mechanisms initially superimpose each other but dissipate at different stages due to their different kinetic rates.

Carina Wismeth

Funding
TUM IGSSE

Cooperation
Prof. Manhart, Chair of Hydromechanics, TUM

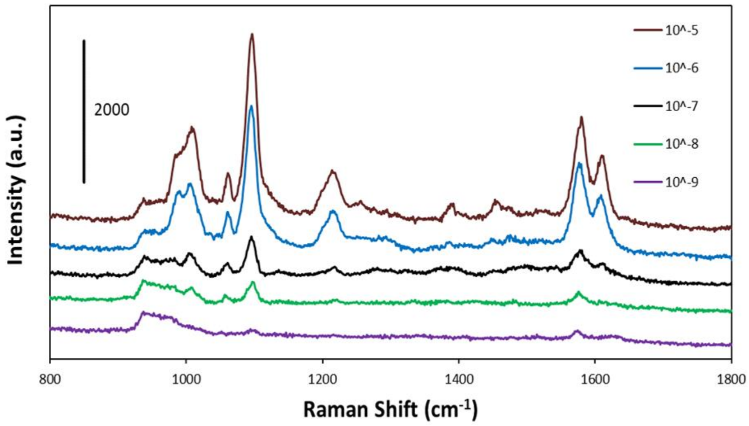
Fabrication of Au@Ag nanoparticles-coated silicon wafer as surface-enhanced Raman scattering (SERS) substrate

Abstract: SERS is considered to be a very powerful analytical method gaining a wide application prospect in sensitive detection of low concentration analytes.

State of the Art. Surface-enhanced Raman Scattering (SERS) is a technique which overcomes the low sensitivity of normal Raman spectroscopy while maintaining the chemical selectivity and has been widely used to detect molecules in low concentrations. The fabrication of SERS substrates is one of the key processes for SERS analysis

5×10^{-5}
5×10^{-6}
5×10^{-7}
5×10^{-8}
5×10^{-9}

Analytical Approach. Reproducibility and stability of SERS measurements can be increased by using immobilized SERS substrates that are bound to an easy available material to produce a practical analytical tool. Various materials such as glass, adhesive tape, filter paper and cotton swab have been used to prepare SERS substrates to transform SERS technique into a practical analytical tool. Here, we have used a simple electrostatic self-assembly method to prepare Ag@Au coated silicon wafer as SERS substrate. We used silicon wafer due to its good chemical stability and high-purity monocrystal containing a distinct Raman peak at 521 cm^{-1}. The Ag@Au core-shell nanoparticles were deposited on the silicon wafer by using poly (diallyldimethylammonium) (PDDA) as an ordinary positively charged polyelectrolyte.



SERS spectra collected by using the Ag@ Au coated silicon wafer for 4-MPY solutions of different concentrations.

Results. 4-mercaptobenzoic acid (4-MBA) and 4-mercptopyridine (4-MPY) were used as the probe analytes to evaluate the SERS performance including sensitivity, uniformity, reproducibility and stability of the as-prepared substrate. The SERS measurements show detection limits of 5 $\times10^{-9}$ M for both selected molecules. Furthermore, the uniformity and stability of this substrate have been studied and the results are satisfactory. The fabrication process is easy to handle and the as-prepared substrate is ideal for the detection of selected molecules in environmental samples like tap and snowmelt water.

Sayed Amininejad, Natalia P. Ivleva, Thomas Baumann

References

(1) Wang, N.; Ma, Z.; Zhou, S.; Liang, G., Facile fabrication of SERS substrate based on food residue eggshell membrane. Chemical Physics Letters. 2016, 666, 45-50.

Funding
DFG
Cooperation
Research Unit Internano

Scalings in geothermal facilities

Scalings are a widespread problem among geothermal plants which exploit the Malm Aquifer in the Bavarian Molasse Zone. They effect the technical and economic efficiency of geothermal plants.

State of the Art. The majority of the scalings observed at geothermal facilities exploring the Malm Aquifer in the Bavarian Molasse Basin are carbonates. They are formed due to a disruption of the lime-carbonic-acid equilibrium during production caused by degassing of CO_2. These scalings are found in the production pipes, at the pumps, and at filters and can nicely be described using existing hydrogeochemical models.

Analytical Approach. In order to mitigate those scalings, the process of scaling formation and the influencing factors have to be better understood. Therefore, scalings of all sections of geothermal facilities have been taken. The database consists of scaling samples from 13 geothermal pumps, 6,000 m production pipe (sample interval 10-12 m), 11 evaporator revisions, 2 injection pipes and numerous filter elements. The samples were analysed by SEM-EDX, XRD, Raman spectroscopy and acid digestion to assess their chemical and mineralogical composition.

Results. The scalings mainly consist of calcium carbonate with traces of incorporated magnesium (0.5-2.0 wt%). At the pipe side of the carbonate scalings a thin initial layer consists of either iron sulfide or copper sulfide depending on the substrate material. Particularly at the groundlevel facilities, but also in the upper part of the production pipe, thin layers of apatite were found at facilities which regularly clean their pipes with phosphoric acid. While the precipitation of apatite during application of phosphoric acid is not likely due to the low pH-value, remnants of phosphor ions remain in the pipes and may later crystallise to apatite during neutralisation with tap water before the geothermal production is resumed.

Coarse- crystalline scaling formed in a production pipe with a smooth polymer coating. Due to the poor cohesion, scalings get easily detached and get washed into the filters which eventually leads to blocking of the filters.

The scaling thickness distribution along the production pipes together with operational data allow an estimate of the average scaling rate for each depth, which is rising from bottom to top. At the well head, the investigated sites exhibit calcium carbonate scaling rates in the range of $1.5\text{-}4.0 \cdot 10^{-6}$ mol/ (m^2*s).

The scalings in the production pipes usually do not present a serious problem in geot hermal facilities exploring the carbonates in the Molasse Basin, as long as they are not mobilized. The pressure drop ist almost neglible. In contrast mobilized scalings can cause a shutdown. An oil film in the surface level facilities, as observed in several facilities, increases the risk for an accumulation of scaling fragments at heat exchangers and valves.

Bernhard Köhl, Thomas Baumann

Funding

Geothermie-Allianz Bayern

Cooperation

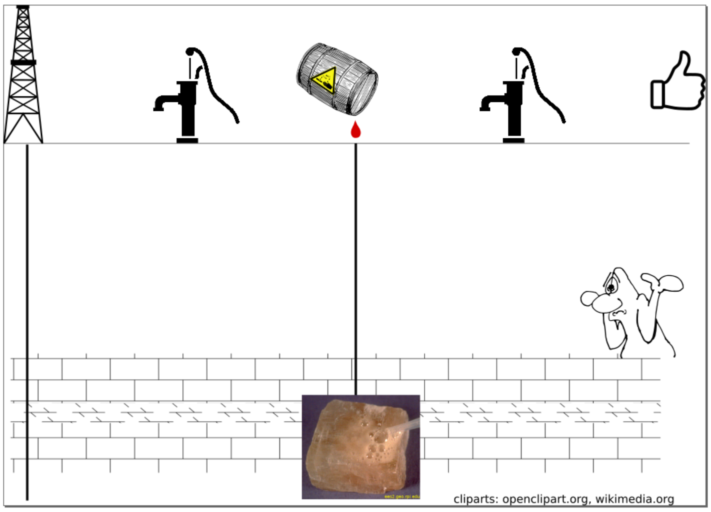
Operators of geothermal facilities in the Bavarian Molasse Basin

Stadtwerke München

Hydrochemical Monitoring and Thermo-Hydraulic-Chemical Modelling

Is it possible to gain useful information about the matrix properties of a deep carbonatic reservoir by evaluating the development of the acid concentration after chemical stimulation during exploration?

Motivation During exploration of a geothermal system, chemical stimulation using inorganic acid is conducted to improve the permeability from the aquifer matrix to the borehole and to remove drilling mud in the vicinity of the borehole. These stimulation processes are repeated two to three times. The idea of this project is, to monitor the produced fluid after chemical stimulation to gain information about the hydraulic development of the flow paths and to predict the long term behaviour of the well.



Sketch of the acid stimulation of the reservoir.

Analytical Approach Acid stimulation of the Malm aquifer is mainly operated by injecting hydrochlorid acid into the aquifer. The development of the chloride ion concentration over the produced water volume shows the dispersion of the acid in the vicinity of the borehole. In the first part of the project, ion concentrations of selected elements were analysed from different construction sites. These sites were spatially scattered across the Malm aquifer of the Bavarian Molasse Basin. Currently the database holds monitoring data from six stimulation steps. A mass balance and the dissolved volume of aquifer matrix was estimated by using calcite and dolomite concentrations calculated with the software programm PhreeqC.

Results Five of these drilling sites were successful with production rates exceeding 50 L/s, while another well was below 5 L/s. The chloride ion concentrations show a biexponential decrease with increasing produced volume. The first part with rapidly decreasing concentrations is representative for the water produced from the borehole and from larger fractures and joints. In the second part the concentrations are decreasing more slowly. This is representative for water produced from the matrix. In all cases the coefficients of the two exponentials became closer to each other after the second acid application. This indicates that the flow pattern in the vicinity of the borehole is getting more homogeneous, i.e., small flow paths in the matrix are widened and the connection of the borehole to the matrix is improved. It also suggests that additional acid applications will most likely be less effective. The dissolved volumes depend on the location but are in the range of some tons rock matrix per acidification step.

Thomas Baumann, Martina Ueckert

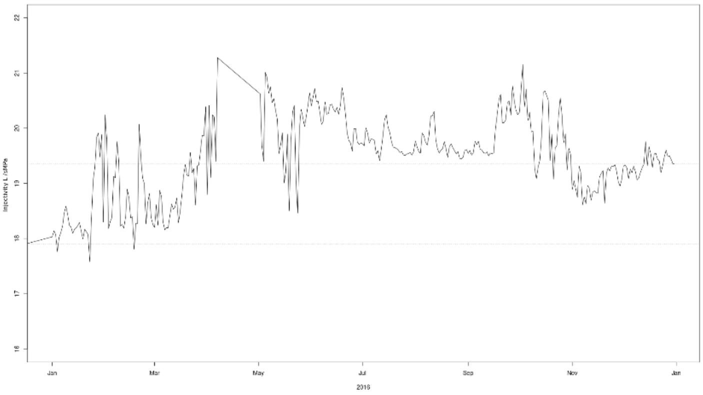
Funding
Bavarian State Ministry of Economy

Cooperation
J. Bartels, Aquasoil GmbH

Large-Scale Geothermal Exploration of the Bavarian Molasse Basin

Coupling of geothermal power plant systems running at high temperatures in the south of Munich with district heating systems in the north of Munich might increase the efficiency of heat mining.

Motivation The Malm aquifer of the Bavarian Molasse Basin is dipping towards the Alps and consequently higher temperatures show up in the southern part of Munich compared to the northern part. The idea is, to use the boreholes in the south to produce hot water and to pump that water via a district heating system into the north of Munich. The heat is extracted along the way and the cooled water is then injected into, now two, injection wells in the north. That results in an increase in efficiency of about 70 %. However, producing water in the south with flow rates of more than 100 L/s and injecting it 30 km in the north may induce large-scale hydraulic changes or even trigger seismic events. We are investigating issues caused by hydrogeochemical changes. The mixing of different water compositions which contain gas and potentially oil phases will affect the plant components as well as the aquifer matrix .



Injectivity at the injection well in the north during one year.

The Model Data from the operational geothermal dublet system in the south and in the north were used to establish a conceptual model with PhreeqC. Using this model, hydrogeochemical reactions can be predicted and quantified, which is crucial for planning operation.

Results Evaluating monitoring data from the geothermal dublet system in the north proves an increase of injectivity during one year. Besides thermo-hydraulic oscillation also hydrogeochemical effects can be seen. Even at the current, rather low temperature spread of 10-20 °C, dissolution of the aquifer matrix leads to a moderate increase of injectivity. Within this research project, water from a different lithostratigraphic setting and with much higher initial temperatures will be produced and after heat extraction ($\Delta T \sim 65$ °C) it will be strongly undersaturated with respect to the carbonatic mineral phases. Producing this 130 °C hot water from the south and cooling it down to 65 °C will result in a saturation index for calcite of -0.85 and for dolomite of -2.13. Taken the slower reaction rates of dolomite into account, it will still result in a strong dissolution of the aquifer matrix, indicating a total volume of about 0.2 m³ calcite and dolomite per day. The dissolution will occur in the vicinity of the borehole and the injectivity will significantly increase.

Thomas Baumann, Martina Ueckert

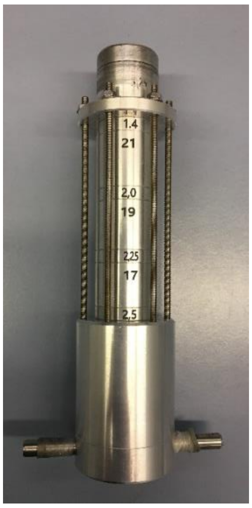
Funding
BayMWi; Exorka GmbH

Cooperation
Exorka GmbH; LIAG

The Mechanical Workshop

Many of our activities, single experiments, field campaigns, and even complete projects would be impossible without our excellent mechanical workshop. While it is called a mechanical workshop, they do much more than producing precision mechanic parts: construction of components and even complete instruments, design and development of electronics, programming of our newly developed instruments and more. Just see some examples here:

Aerodynamic Lens An aerodynamic lens is a device used to concentrate aerosol particles in a gas stream. We use such lens to increase the sensitivity of our new Laser-Induced Breakdown Spectroscopy (LIBS) aerosol analysis device (which to a large part was also build by our workshop).

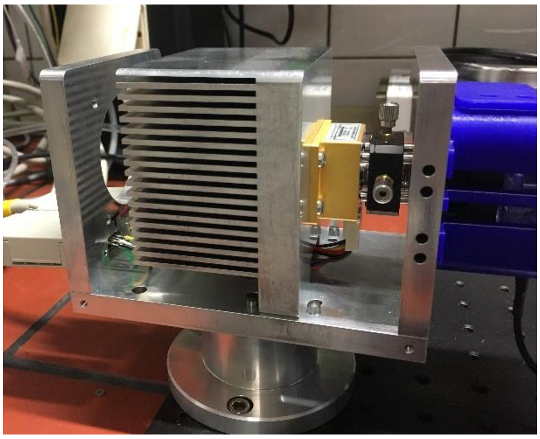


Aerodynamic lens to focus particles in an aerosol flow for a more efficient detection by LIBS.

Mobil Mass Spectrometer. Our new HELIOS/SICRIT mass spectrometry system would have been possible without the workshop. The HELIOS evaporation system is machined from a massive block of stainless steel. The complete system including MS and pumps was integrated into two mobile racks, 1 m^3 each, which makes the system highly mobile and robust. It takes less than 30 min from the trunk of the car to full operation.

the complete HELIOS/SICRIT/MS on a chassis dyno.

Quantum Cascade Laser. For various photoacoustic instruments, we use quantum cascade lasers (QCLs). The workshop built the complete mount and the adjustments, including the optical beam steering.



Our workshop magicians: Sebastian Wiesemann and Hoppe

Publications

Peer-Reviewed Journals

Anger, P. M.*; von der Esch, E.*; Baumann, T.; Elsner, M.; Niessner, R.; Ivleva, N. P., Raman microspectroscopy as a tool for microplastic particle analysis. *TrAC Trends in Analytical Chemistry* 2018, *109*, 214-226. (* shared first authorship)
https://doi.org/10.1016/j.trac.2018.10.010

Bakkour, R.; Bolotin, J.; Sellergren, B.; Hofstetter, T. B., Molecularly imprinted polymers for compound-specific isotope analysis of polar organic micropollutants in aquatic environments. *Analytical Chemistry* 2018, *90*, (12), 7292-7301.
https://doi.org/10.1021/acs.analchem.8b00493

Beloglazova, N. V.; Lenain, P.; De Rycke, E.; Goryacheva, I. Y.; Knopp, D.; De Saeger, S., Capacitive sensor for detection of benzo(a)pyrene in water. *Talanta* 2018, *190*, 219-225.
https://doi.org/10.1016/j.talanta.2018.07.084

Bemetz, J.; Wegemann, A.; Saatchi, K.; Haase, A.; Häfeli, U. O.; Niessner, R.; Gleich, B.; Seidel, M., Microfluidic-based synthesis of magnetic nanoparticles coupled with miniaturized NMR for online relaxation studies. *Analytical Chemistry* 2018, *90*, (16), 9975-9982.
https://doi.org/10.1021/acs.analchem.8b02374

Degenkolb, L.; Metreveli, G.; Philippe, A.; Brandt, A.; Leopold, K.; Zehlike, L.; Vogel, H.-J.; Schaumann, G. E.; Baumann, T.; Kaupenjohann, M.; Lang, F.; Kumahor, S.; Klitzke, S., Retention and remobilization mechanisms of environmentally aged silver nanoparticles in an artificial riverbank filtration system. *Science of The Total Environment* 2018, *645*, 192-204.
https://doi.org/10.1016/j.scitotenv.2018.07.079

Dina, N. E.; Gherman, A. M. R.; Chiş, V.; Sârbu, C.; Wieser, A.; Bauer, D.; Haisch, C., Characterization of clinically relevant fungi via SERS fingerprinting assisted by novel chemometric models. *Analytical Chemistry* 2018, *90*, (4), 2484-2492.
https://doi.org/10.1021/acs.analchem.7b03124

Domogalla-Urbansky, J.; Anger, P. M.; Ferling, H.; Rager, F.; Wiesheu, A. C.; Niessner, R.; Ivleva, N. P.; Schwaiger, J. J. E. S.; Research, P., Raman microspectroscopic identification of microplastic particles in freshwater bivalves (Unio pictorum) exposed to sewage treatment plant effluents under different exposure scenarios. 2019, *26*, (2), 2007-2012.
https://doi.org/10.1007/s11356-018-3609-3

Ehrl, B. N.; Gharasoo, M.; Elsner, M., Isotope fractionation pinpoints membrane permeability as a barrier to atrazine biodegradation in gram-negative *Polaromonas sp.* Nea-C. *Environmental Science & Technology* 2018, *52*, (7), 4137-4144.
https://doi.org/10.1021/acs.est.7b06599

Ehrl, B. N.; Mogusu, E. O.; Kim, K.; Hofstetter, H.; Pedersen, J. A.; Elsner, M., High Permeation Rates in Liposome Systems Explain Rapid Glyphosate Biodegradation Associated with Strong Isotope Fractionation. *Environmental Science & Technology* 2018, *52*, (13), 7259-7268.
https://doi.org/10.1021/acs.est.8b01004

Elsäßer, D.; Ho, J.; Niessner, R.; Tiehm, A.; Seidel, M., Heterogeneous asymmetric recombinase polymerase amplification (haRPA) for rapid hygiene control of large-volume water samples. *Analytical Biochemistry* 2018, *546*, 58-64.
https://doi.org/10.1016/j.ab.2018.01.032

Gafni, A.; Lihl, C.; Gelman, F.; Elsner, M.; Bernstein, A., δ13C and δ37Cl isotope fractionation to characterize aerobic vs anaerobic degradation of trichloroethylene. *Environmental Science & Technology Letters* 2018, *5*, (4), 202-208.
https://doi.org/10.1021/acs.estlett.8b00100

Goettel, M.; Niessner, R.; Scherer, M.; Scherer, G.; Pluym, N., Analysis of urinary eicosanoids by LC–MS/MS reveals alterations in the metabolic profile after smoking cessation. *Chemical Research in Toxicology* 2018, *31*, (3), 176-182.
https://doi.org/10.1021/acs.chemrestox.7b00276

Heckel, B.; McNeill, K.; Elsner, M., Chlorinated ethene reactivity with vitamin B12 is governed by cobalamin chloroethylcarbanions as crossroads of competing pathways. *ACS Catalysis* 2018, *8*, (4), 3054-3066.
https://doi.org/10.1021/acscatal.7b02945

Hörbrand, T.; Baumann, T.; Moog, H. C. J. G. E., Validation of hydrogeochemical databases for problems in deep geothermal energy. 2018, *6*, (1), 20.
https://doi.org/10.1186/s40517-018-0106-3

Imhof, H. K.; Wiesheu, A. C.; Anger, P. M.; Niessner, R.; Ivleva, N. P.; Laforsch, C., Variation in plastic abundance at different lake beach zones - A case study. *Science of The Total Environment* 2018, *613-614*, 530-537.
https://doi.org/10.1016/j.scitotenv.2017.08.300

Kah, M.; Sigmund, G.; Manga Chavez, P. L.; Bielská, L.; Hofmann, T., Sorption to soil, biochar and compost: is prediction to multicomponent mixtures possible based on single sorbent measurements? *PeerJ* 2018, 6, e4996.
https://doi.org/10.7717/peerj.4996

Kober, C.; Niessner, R.; Seidel, M., Quantification of viable and non-viable Legionella spp. by heterogeneous asymmetric recombinase polymerase amplification (haRPA) on a flow-based chemiluminescence microarray. *Biosensors and Bioelectronics* 2018, *100*, 49-55.
https://doi.org/10.1016/j.bios.2017.08.053

Massner, C.; Sigmund, F.; Pettinger, S.; Seeger, M.; Hartmann, C.; Ivleva, N. P.; Niessner, R.; Fuchs, H.; de Angelis, M. H.; Stelzl, A.; Koonakampully, N. L.; Rolbieski, H.; Wiedwald, U.; Spasova, M.; Wurst, W.; Ntziachristos, V.; Winklhofer, M.; Westmeyer, G. G., Genetically controlled lysosomal entrapment of superparamagnetic ferritin for multimodal and multiscale imaging and actuation with low tissue attenuation. *Advanced Functional Materials* 2018, *28*, (19), 1706793.
https://doi.org/10.1002/adfm.201706793

Melnik, S.; Neumann, A.-C.; Karongo, R.; Dirndorfer, S.; Stübler, M.; Ibl, V.; Niessner, R.; Knopp, D.; Stoger, E., Cloning and plant-based production of antibody MC10E7 for a lateral flow immunoassay to detect [4-arginine]microcystin in freshwater. *Plant Biotechnol J.* 2018, *16*, (1), 27-38.
https://doi.org/10.1111/pbi.12746

Moreno-Paz, M.; Gómez-Cifuentes, A.; Ruiz-Bermejo, M.; Hofstetter, O.; Maquieira, Á.; Manchado, J.M.; Morais, S.; Sephton, M.A.; Niessner, R.; Knopp, D.; Parro, V., Detecting nonvolatile life- and nonlife-derived organics in a carbonaceous chondrite analogue with a new multiplex immunoassay and its relevance for planetary exploration. *Astrobiology* 2018, *18*, (8), 1041-1056.
https://doi.org/10.1089/ast.2017.1747

Nießner, R., Analytische Chemie – aktuelle Trends im Vergleich zu den historischen Anfängen. 2018, *130*, (44), 14524-14533.
https://doi.org/10.1002/ange.201802336

Niessner, R., Analytical chemistry: Current trends in light of the historic beginnings. 2018, *57*, (44), 14328-14336.
https://doi.org/10.1002/anie.201802336

Rodríguez-Fernández, D.; Heckel, B.; Torrentó, C.; Meyer, A.; Elsner, M.; Hunkeler, D.; Soler, A.; Rosell, M.; Domènech, C., Dual element (CCl) isotope approach to distinguish abiotic reactions of chlorinated methanes by Fe(0) and by Fe(II) on iron minerals at neutral and alkaline pH. *Chemosphere* 2018, *206*, 447-456.
https://doi.org/10.1016/j.chemosphere.2018.05.036

Sigmund, G.; Jiang, C.; Hofmann, T.; Chen, W., Environmental transformation of natural and engineered carbon nanoparticles and implications for the fate of organic contaminants. *Environmental Science: Nano* 2018, *5*, (11), 2500-2518.
https://doi.org/10.1039/C8EN00676H

Sessa, C.; Weiss, R.; Niessner, R.; Ivleva, N. P.; Stege, H., Towards a surface enhanced raman scattering (SERS) spectra database for synthetic organic colourants in cultural heritage. The effect of using different metal substrates on the spectra. *Microchemical Journal* 2018, *138*, 209-225.
https://doi.org/10.1016/j.microc.2018.01.009

Steinke, N.; Rio, M.; Wuchrer, R.; Schuster, C.; Ljasenko, E.; Knopp, D.; Gerlach, G.; Härtling, T., Detection of diclofenac molecules by planar and nanostructured plasmonic sensor substrates. *Sensors and Actuators B: Chemical* 2018, *254*, 749-754.
https://doi.org/10.1016/j.snb.2017.07.123

Suwandhi, L.; Hausmann, S.; Braun, A.; Gruber, T.; Heinzmann, S. S.; Gálvez, E. J. C.; Buck, A.; Legutko, B.; Israel, A.; Feuchtinger, A.; Haythorne, E.; Staiger, H.; Heni, M.; Häring, H.-U.; Schmitt-Kopplin, P.; Walch, A.; Cáceres, C. G.; Tschöp, M. H.; Rutter, G. A.; Strowig, T.; Elsner, M.; Ussar, S., Chronic d-serine supplementation impairs insulin secretion. *Molecular Metabolism* 2018, *16*, 191-202.
https://doi.org/10.1016/j.molmet.2018.07.002

Thaler, K. M.; Schwartz, A. J.; Haisch, C.; Niessner, R.; Hieftje, G. M., Preliminary survey of matrix effects in the Microwave-sustained, Inductively Coupled Atmospheric-pressure Plasma (MICAP). *Talanta* 2018, *180*, 25-31.
https://doi.org/10.1016/j.talanta.2017.12.021

Torrentó, C.; Prasuhn, V.; Spiess, E.; Ponsin, V.; Melsbach, A.; Lihl, C.; Glauser, G.; Hofstetter, T. B.; Elsner, M.; Hunkeler, D., Adsorbing vs. nonadsorbing tracers for assessing pesticide transport in arable soils. 2018, *17*, (1).
http://doi.org/10.2136/vzj2017.01.0033

Wiesheu, A. C.; Brejcha, R.; Mueller, C. W.; Kögel-Knabner, I.; Elsner, M.; Niessner, R.; Ivleva, N. P. J. A.; Chemistry, B., Stable-isotope Raman microspectroscopy for the analysis of soil organic matter. 2018, *410*, (3), 923-931.
https://doi.org/10.1007/s00216-017-0543-z

Wunderlich, A.; Heipieper, H. J.; Elsner, M.; Einsiedl, F., Solvent stress-induced changes in membrane fatty acid composition of denitrifying bacteria reduce the extent of nitrogen stable isotope fractionation during denitrification. *Geochimica et Cosmochimica Acta* 2018, *239*, 275-283.
https://doi.org/10.1016/j.gca.2018.07.037

Yang, D.; Zhou, H.; Dina, N. E.; Haisch, C., Portable bacteria-capturing chip for direct surface-enhanced Raman scattering identification of urinary tract infection pathogens. 2018, *5*, (9), 180955.
https://doi.org/10.1098/rsos.180955

Yuan, K.; Mei, Q.; Guo, X.; Xu, Y.; Yang, D.; Sánchez, B. J.; Sheng, B.; Liu, C.; Hu, Z.; Yu, G.; Ma, H.; Gao, H.; Haisch, C.; Niessner, R.; Jiang, Z.; Zhou, H., Antimicrobial peptide based magnetic recognition elements and Au@Ag-GO SERS tags with stable internal standards: a three in one biosensor for isolation, discrimination and killing of multiple bacteria in whole blood. *Chemical Science* 2018, *9*, (47), 8781-8795.
http://doi.org/10.1039/C8SC04637A

Non Peer-Reviewed

N. P. Ivleva, How to detect microplastics. *Analytica Pro* 2018, 1, 14-18

Conference Presentations

Oral Presentations

Anger, P. M.; Niessner, R.; Elsner, M.; Ivleva, N. P., Towards (semi-)automation of microplastic analysis by means of Raman microspectroscopy. *6IMDC 2018*, 12.-16.3.2018, San Diego, USA.

Anger, P. M.; Niessner, R.; Elsner, M.; Ivleva, N. P., Optimization and automation of Raman microspectroscopy for microplastic analysis. *WASSER 2018*, 7.-9.5.2018, Papenburg, Germany.

Anger, P. M.; Niessner, R.; Elsner, M.; Ivleva, N. P., Optimization and automation of Raman microspectroscopy for microplastic analysis. *SETAC Europe 2018*, 13.-17.5.2018, Rom, Italy.

Ivleva, N. P., Microplastic in environmental samples: Identification and quantification by Raman microspectroscopy. *MicroPlastics2018*, 28.-31.0.2018, Monte Verita, Ascona, Switzerland (invited)

Ivleva, N. P., SERS in Combination with stable isotope approach for analysis of bacteria at single cell level. *SciX 2018*, 21.-26.10.2018, Atlanta, USA, (invited)

Ivleva, N. P., Stable isotope Raman microspectroscopy for environmental analysis: Feasibility studies. *Analytica conference 2018, New Developments in Analytical Spectroscopy – The Power of Light*, 10.-13.4.2018, Munich, Germany (invited)

Ivleva, N. P., Identification and quantification of microplastic: Focus on Raman microspectroscopic analysis. *Analytica conference 2018, Analysis of Microplastics,* 10.-13.4.2018, Munich, Germany (invited)

von der Esch, E.; Zinterhof, P.; Anger, P. M.; Elsner, M.; Niessner, R.; Ivleva, N. P., Roadmap towards automated Raman microscopy of microplastic. *UMWELT 2018*. 09.-12.9.2018, Münster, Germany.

Schwaferts, C.; Niessner, R.; Elsner, M.; Ivleva, N. P., Raman-Mikrospektroskopie von Submikrometer-Plastikpartikeln. *UMWELT 2018*, 10.-12.9.2018, Münster, Germany

Wismeth, C.; Glaubitz, C.; Manhart, M.; Elsner M.; Baumann, T., Characterization of interfacial convection in microfluidic systems. *EGU General Assembly*, 8.-13.4.2018, Vienna, Austria.

Wieland, C.; Seitz-Gutmann, A.; Spliethoff, H.; Baumann, T., CO_2 -neutrale Begleitgasnutzung in tiefengeothermischen Anlagen. *Der Geothermie Kongress*, 27.-29.11.2018, Essen, Germany.

Ueckert, M.; Baumann, T., Großräumige geothermische Nutzung im Bayerischen Molassebecken. *Der Geothermie Kongress*, 27.-29.11.2018, Essen, Germany.

Kurtz, S.; Metreveli, G.; Klitzke, S.; Seitz, F.; Rosenfeldt, R. R.; Lüderwald, S.; Baumann, T.; Bundschuh, M.; Manz, W.; Schulz, R.; Vogel, H.-J.; Schaumann, G. E., Distribution of Ag and TiO_2 nanoparticles in aquatic-terrestrial indoor mesocosm system. *InterNano Conference*, 19.-21.9.2018, Landau, Germany.

Baumann, T.; Ueckert, M.; Hörbrand, T., Hydrogeochemical modelling of aquifer heat storage systems. *26. Tagung FH-DGGV*, 21.-24.3.2018, Bochum, Germany.

Baumann, T.; Ueckert, M.; Bartels, J., Fluidmonitoring nach Stimulationsmaßnahmen und TH*C*M. *Der Geothermie Kongress*, 27.-29.11.2018, Essen, Germany.

Baumann, T.; Köhl, B., Scalings - Past, Present and Future. *Der Geothermie Kongress*, 27.-29.11.2018, Essen, Germany.

Aminineyad, S.; Ivleva, N. P.; Baumann, T., Surface-enhanced Raman scattering (SERS) for characterization of coatings on metallic nanoparticles. *InterNano Conference*, 19.-21.9.2018, Landau.

Seidel, M., Schnellanalyse von organischen Spurenstoffen und antibiotikaresisten Bakterien. *Abwasserkolloquium 2018*, 8.11.2018, Stuttgart, Germany.

Seidel, M., Analytical microarrays for the rapid quantification of antibiotics, antibiotic-resistant bacteria and pathogens. *Adlershofer Kolloquium der Bundesanstalt für Materialforschung und -prüfung und (BAM)*, 6.11.2018, Berlin, Germany.

Göpfert, L.; Elsner, M.; Seidel, M., DNA microarrays for the culture-independent detection of extended-spectrum beta-lactamase genes and bacterial pathogens. *Medical Biodefense Conference 2018*, 28.-31.10.2018, Munich, Germany.

Sollweck, K.; Seidel, M., Development of detection methods for mycotoxin producers and mycotoxins in indoor air. *Medical Biodefense Conference 2018*, 28.-31.10.2018, Munich, Germany.

Seidel, M., Mikroarray-basierte Schnellmesstechnik zur Quantifizierung von organischen Spurenstoffen, Antibiotika-resistenten Keimen und Pathogenen im Wasserkreislauf. *SUK 2018: Spurenstoffe und Krankheitserreger im Wasserkreislauf*, 23.-24.10.2018, Frankfurt, Germany.

Seidel, M., Kulturunabhängige Detektionsmethoden zur Quantifizierung von pathogenen Bakterien und Viren im Wasser. *3. Mülheimer Wasseranalytisches Seminar*, Mülheim, Germany.

Seidel, M., Flow-based chemiluminescence microarrays as tool for rapid detection of pathogens and toxins. *XVIIIth International Symposium on Luminescence Spectrometry*, 18.-22.6.2018, Brest, France.

Kober, C.; Gründel, A.; Bemetz, J.; Petzold, M.; Zamfir, M.; Herr, C.; Lück, C.; Niessner, R.; Seidel, M., LegioTyper: The microarray-based and automated detection method for the rapid serotyping of *Legionella pneumophila* in water and urine samples. *Wasser 2018*, 9.5.2018, Papenburg, Germany.

Seidel, M., Rapid methods for the quantification of pathogenic bacteria and viruses in water. *EU WaterSpy Workshop*, 3.4.2018, Vienna, Austria.

Bemetz, J.; Kober, C.; Niessner, R.; Seidel, M., Flow-based chemiluminescence microarrays with multilayer plastic foils: cheap, simple, universally applicable. *ABC-Spotlight on Bio- and Environmental Analysis*, 11.4.2018, Munich, Germany.

Seidel, M., Multilayer plastic foils for simple flow-based microanalytical systems. *Seminar at Institut für Analytische und Bioanalytische Chemie*, 13.3.2018, Ulm, Germany.

Poster Presentations

Anger, P. M.; Niessner, R.; Elsner, M.; Ivleva, N. P., Improved and automated Raman microspectroscopic analysis of microplastic, *Analytica Conference*, 10.-13.4.2018, Munich, Germany.

Amininejad, S.; Ivleva, N. P.; Baumann, T., Application of surface-enhanced Raman scattering for detection of coatings on Au@Ag nano particles. *Wasser 2018*, 7.-9.2018, Papenburg, Germany.

Amininejad, S.; Ivleva, N. P.; Baumann, T., Analysis of coatings on Au@Ag nanoparticles using surface-enhanced Raman spectroscopy (SERS). *EGU General Assembly*, 8.-13.4.2018, Vienna, Austria.

Bakkour, R.; Vogler, B.; Salhi, E.; Singer, H.; Hofstetter, T. B., Water-compatible molecularly-imprinted polymers enable carbon isotope analysis of glyphosate and AMPA in aquatic environments. *ASI-Jahrestagung* 2018, 30.09 - 03.10.2018, Burghausen, Germany.

Bemetz, J.; Wegemann, A.; Gleich, B.; Niessner, R.; Seidel, M., Miniaturized relaxometer for process monitoring in the microfluidic flow-synthesis of magnetic nanoparticles. *Analytica Conference 2018*, 10.-13.04.2018, Munich, Germany.

Bemetz, J.; Wegemann, A.; Kober, C.; Gleich, B.; Niessner, R.; Seidel, M., Detection of *Legionella pneumophila* in porous monolithic filters by a miniaturized nuclear magnetic resonance system, *12th International Conference on the Scientific and Clinical Applications of Magnetic Carriers*, May 2018, Copenhagen, Denmark.

Degenkolb, L.; Lang, F.; Metreveli, G.; Klitzke, S.; Philippe, A.; Zehlike, L.; Brandt, A.; Leopold, K.; Kumahor, S.; Schaumann, G. E.; Baumann, T.; Vogel, H. J.; Kaupenjohann, M., Die Alterung von Silbernanopartikeln in Böden erhöht ihre Mobilität und ihr Remobilisierungspotential in der Uferfiltration. *Wasser 2018*, 7.-9.2018, Papenburg, Germany.

Elsner, M.; Ehrl, B.; Kundu, K.; Marozova, S; Gharasoo, M.; Rate-limiting mass transfer in micropollutant degradation revealed by isotope fractionation, *Gordon Research Conference Environmental Sciences: Water,* 24.-29.6.2018, Holderness, U.S.

Glöckler, D.; Bakkour, R.; Wabnitz, C.; Sigmund, G.; Seidel, M.; Elsner, M., Graphene-modified polymer monoliths for high throughput extraction of micropollutants for compound-specific isotope analysis. *ASI-Jahrestagung* 2018, 30.09 - 03.10.2018, Burghausen, Germany

Göpfert, L.; Calomfirescu, D.; Höller, C.; Elsner, M.; Seidel, M., Comparison of DNA Microarrays with PCR for the Detection of Extended Spectrum beta-Lactamase gene CTX-M. *Analytica Conference*, 2018, 10.-12.4.2018, Munich, Germany.

Göpfert, L.; Calomfirescu, D.; Höller, C.; Elsner, M.; Seidel, M., Detection of CTX-M Extended Spectrum beta Lactamase (ESBL) in Pathogenic Bacteria from Surface Waters using the Heterogeneous Asymmetric Recombinase Polymerase Amplification (haRPA). *Tagung Wasser 2018*, 7.-9.5.2018, Papenburg, Germany.

Hartmann, C.; Pettinger, S.; Massner, C.; Elsner, M.; Westmeyer, G.; Niessner, R.; Ivleva, N.P., Raman Analysis of Iron-containing Proteins. *Analytica Conference 2018*, 10.-13.4.2018, Munich, Germany.

Kober, C.; Gründel, A.; Bemetz, J.; Petzold, M.; Zamfir, M.; Herr, C.; Lück, C.; Niessner, R.; Seidel, M., Culture-independent Serotyping of *Legionella pneumophila* in Water and Urine Samples for Faster Risk Assessment of Legionella Expositions. *Analytica Conference 2018*, 10.-13.04.2018, Munich, Germany.

Kober, C.; Gründel, A.; Bemetz, J.; Petzold, M.; Zamfir, M.; Herr, C.; Lück, C.; Niessner, R.; Seidel, M., Culture-independent Serotyping of L. pneumophila in Water and Urine Samples for Faster Risk Assessment of Legionella Exposures. *16th Medical Biodefense Conference*, 28.-31.10.2018, Munich, Germany.

Kober, C.; Niessner, R.; Seidel, M., Microarray-based rapid verification and risk assessment of viable Legionella by on-chip amplification. *16th Medical Biodefense Conference*, 28.-31.10.2018, Munich, Germany.

Köhl, B.; Baumann, T., Scalings at geothermal facilities - characterization, processes and mass balance. *EGU General Assembly*, 8.-13.4.2018, Vienna, Austria.

Morgaienko, O.; Marozava, S.; Elsner, M.; Ivleva, N. P., Coupling of BONCAT (bioorthogonal noncanonical amino acid tagging) and SERS (surface enhanced Raman scattering) for analysis of bacteria degrading organic pollutants. *Analytica conference 2018*, 10-12.04.2018, Munich, Germany.

Morgaienko, O.; Elsner, M.; Ivleva, N. P., Development of bioorthogonal noncanonical amino acid tagging – surface enhanced Raman scattering to visualize bacteria responsible for degradation of organic pollutants. *WASSER 2018*, 7.-9.05.2018, Papenburg, Germany.

Schwaferts, C.; Niessner, R.; Elsner, M.; Ivleva, N. P., Detection and identification of submicrometerplastic particles using Raman microspectroscopyand scanning electron microscopy. *Analytica Conference*, 10.-13.4.2018, Munich, Germany.

Schwaferts, C.; Niessner, R.; Elsner, M.; Ivleva, N. P., Detektion und Identifizierung von Sub µ-Plastikpartikeln mit Raman-Mikrospektroskopie. *WASSER 2018*, 7.-9.5.2018, Papenburg, Germany.

Sigmund, G.; Marozava, S.; Sun, F.; Kundu, K.; Morgaienko, O.; Ivleva, N. P.; Elsner, M., Compound-specific isotope analysis (CSIA) for the investigation of bottlenecks for atrazine degradation with Arthrobacter aurescens TC1 under varying nutrient availabilities. *ASI-Jahrestagung 2018*, 30.09. - 03.10.2018, Munich, Germany.

Ueckert, M.; Baumann, T., Large scale geothermal exploration in the Bavarian Molasse basin. *EGU General Assembly*, 8.-13.4.2018, Vienna, Austria.

von der Esch, E.; Zinterhof, P.; Anger, P. M.; Elsner, M.; Niessner, R.; Ivleva, N. P., Roadmap towards automated Raman microscopy of microplastic. *Witec Symposium 2018*. 24-26.9.2018, Ulm, Germany.

von der Esch, E.; Elsner, M.; Niessner, N.; Ivleva, N. P., Automated characterization of microplastic (bioplastic and conventional) by means of Raman microspectroscopy. *Analytica Conference 2018*. 10-13.4.2018, Munich, Germany.

von der Esch, E.; Elsner, M.; Niessner, R.; Ivleva, N. P., Charakterisierung von Biopolymeren in Umweltproben mittels Raman-Mikrospektroskopie. *WASSER 2018*. 5-7.5.2018, Papenburg, Germany.

Invited Lectures

Baumann, T.; Köhl, B.; Scalings in Geothermal Systems – Past, Present, and Future. *GDMB FA Geothermie*, 7.-8.6.2018, Witten, Germany.

Baumann, T., Hydrogeologie des Oberpfälzer Jura. *Workshop: Grundwasserschutz geht uns alle an*. 8.2.2018, Neumarkt, Germany.

Elsner, M., Advancements in Compound-Specific Isotope Analysis (CSIA): Perspectives for Studying Reaction Mechanisms in Complex Systems. *Bundesanstalt für Materialforschung und -prüfung, BAM,* 6.2.2018.

Elsner, M., Kundu, K.; Ehrl, B. N.; Marozava, S.; Gharasoo, M.; Bottlenecks of Atrazine Degradation: Bioavailability Limitation or Physiological Adaption? *University of Hohenheim,* 14.5.2018

Elsner, M., Advancements in Compound-specific Isotope Analysis (CSIA): Perspectives for Studying Reaction Mechanisms in Complex Systems. *University Duisburg-Essen,* 28.5.2018

Elsner, M., Hoelzer , K.; Plata, D.; Chemistry and Environmental Impact of Hydraulic Fracturing (“Fracking“) Fluids, *Gordon Research Conference on Geochemistry,* 29.7.-3.8.2018, Holderness, U.S.

Elsner, M., Chemikalien beim Hydraulic Fracturing („Fracking“) zur Erdgasgewinnung, *6. E.O. Fischer-Seminar „Umwelt und Energie“ in Burghausen Aventinus Gymnasium Burghausen*, 04.10.2018 , Raitenhaslach, Germany.

Elsner, M., Chemie um uns herum, Experimentalvorlesung, *Technische Universität München, Fakultät für Chemie, Tag der offenen Tür*, 13.10.2018

Haisch, C., Optical and Mass Spectrometry: Topical Applications, *University of Vienna*, 06.12.2018, Vienna, Austria.

Haisch, C., Photoacoustic gas-phase spectroscopy: Fundamentals and applications, *Karlsruher Institut für Technologie (KIT)*, 26.01.2018, Karlsruhe, Germany.

Haisch, C., A two-compartment microbial fuel cells as biosensor, invited lecturer for master course, University of Innsbruck, 11.06.2018, Innsbruck, Austria.

Ivleva, N. P., Mikroplastik in der Umwelt, *6. E.O. Fischer-Seminar „Umwelt und Energie“ in Burghausen Aventinus Gymnasium Burghausen*, 04.10.2018 , Raitenhaslach, Germany.

Scientific Committees & Memberships

Baumann, T., Fate and Transport of Biocolloids and Nanoparticles in Soil and Groundwater, EGU General Assembly, 8.-13.4.2018, Vienna (Convener)

Baumann, T., InterNano Conference, 19.-21.9.2018, Landau (Scientific Committee)

Baumann, T., Workshop Scalings – Monitoring & Forensics, Der Geothermie Kongress, 27.-29.11.2018, Essen (Scientific Committee and Organizer).

Seidel, M., Pathogens and antibiotic resistant bacteria in the water cycle, since November (Chairman of the expert committee at the Wasserchemische Gesellschaft)

Seidel, M., Clean Air Commission in the VDI and DIN: Measurement and environmental health assessment of bioaerosols in ambient air. (Member of the working group *NA134.03.07.09 UA*)

Seidel, M., Bioaerosols and biological agents (Member of the working group *NA 134-03-07-04 UA*)

Seidel, M., Mirror committee CEN/TC 264/WG 28, Microorganisms in ambient air (Member of the working group *NA 134-03-07-03-01 AK*)

Consulting

Bakkour, R.

International Atomic Energy Agency - Expert mission on sampling procedures and sample preparation for compound-specific isotope analysis - pesticides in Slovenian groundwater.

Baumann, T.

Hydrogeological and hydrochemical expertises (mineral water, spa water): Auerbach, Bad Endorf, Bad Birnbach, Fischen, Sibyllenbad, Treuchtlingen, Weißenstadt

Deep Hydrogeothermal Energy Exploration: Aschheim, Geretsried, Munich, Pullach, Waldkraiburg

Elsner, M.

International Atomic Energy Agency – Member of the Research Coordination Panel “Multiple Isotope Fingerprints to Identify Sources and Transport of Agro-Contaminants”.

Mineralization control analyses: Bad Abbach, Bad Aibling, Bad Birnbach, Bad Füssing, Bad Griesbach, Bad Gögging, Bad Reichenhall, Bad Rodach, Bad Wiessee, Bad Wimpfen, Bad Wörishofen, Bayreuth, Erding, Hölle, Kondrau, Neumarkt i. d. Opf., Sibyllenbad, Siegsdorf, Straubing

Haisch, C.

Bavarian companies - Photoacoustic sensor development, on-board emission sensing, and filter characterization.

Theses

PhD Theses

MSc Chem. Benjamin Heckel: Investigating Mechanisms of Reductive Chlorinated Hydrocarbon Degradation with Compound-Specific Isotope Analysis

MSc Chem. Benno Ehrl: Investigating Mass Transfer Limitations during Biodegradaton of Micropollutants with Compound-Specific Isotope Analysis

MSc Chem. Michael Göttel: Analytical Studies on the Impact of Smoking Cessation on the Metabolic Profile

MSc Pharm. Angelika Nistler: Magnetic Nanocomposites for Rapid Biosensing of Staphylococcal Enterotoxin B in Milk

MSc Chem. Alexander Rinkenburger: Die Oxidationsreaktivität von Ruß: Katalytische Beeinflussung durch Kaliumsalze und on-line Charakterisierung

MSc Biochem. Ruoyu Sun: Nanodiscs Incorporating Functional Human Beta-1 Adrenergic Receptors as Novel Diagnostic Approach for Autoimmune Dilated Cardiomyopathy

MSc Chem. Carina Wismeth: Quantitative Parametrisierung der Dynamik konvektiver Rollzellen an Grenzflächen zu nichtwässrigen Phasen in mikrofluidischen Modellen

Dipl.-Geol. Mathias Köster: Tracing fluids involved in the formation of bentonite deposits

M.Sc. Theses

BSc Franziska Adler: Introduction and Validation of a Target-Method for the Detection of Trace Substances Using High-resolution LC-MS/MS Analytics

BSc Jessica Beyerl: Immunological Solid-phase Quantification of Escherichia coli Concentrated by DEAE-functionalized Monolithic Adsorption Filtration (MAF-DEAE) of Tap Water Samples

BSc Christian Biermaier: Polyepoxide Coating of Glass Carriers for the Interaction Analysis of Phages with Functionalized Surfaces

BSc Manjiang Hong: Cross-Flow Monolithic Adsorption Filtration System for Rapid Enrichment of Bacteria in Water

BSc Julia Neumair: Study of Gold Nanoparticle Adsorption on Polyepoxide-based Monoliths Using spICP-MS and SEM

B.Sc. Theses

Nur Aisha Abdul Aziz: Process Monitoring of Flow Synthesis of Coated Magnetic Nanoparticles by Nuclear Magnetic Resonance

Rilette Cirlem Tierra Bautista: Concentration and Analysis of Sulfonamide Antibiotics from Water Samples

Fabian Freire-Moschivitis: Characterization of Interfacial Convections in Microfluidic Systems

Wei Yuan Goh: Elution of Escherichia Coli Concentrated by DEAE-functionalized Monolithic Adsorption Filtration

Sonja Hoffmann: On-line Measurement of Soot Reactivity Using Photoacoustic Spectroscopy

Anna-Lena Holtmannspötter: Mechanistic Investigations of the Reductive Dehalogenation of Dichloromethane with Compound Specific Isotope Analysis

Benedict Horn: Development of a Fast-Gaschromatography-System

Sharon Istvànffy: Optimization of Metal Liquid Like Films and their Application in Surface Enhanced Raman Spectroscopy

Felix Ludwig: Determination of Formaldehyde in OME Fuels

Maximilian Maier: Characterization of a Monoclonal Antibody for the Detection of Pyrrolizidine Alkaloids

Michael Sandholzer: Quantification of Pseudomonas Aeruginosa and CTX-M Genes by Heterogeneous Asymmetric Recombinase Polymerase Amplification

Sabrina Schönberger: Enrichment of Sulfonamides in Water Samples

Sarah Schneidemann: Change in Membrane Fatty Acid Composition During Chemical Pollutant Degradation

Antonia Seitz: Development of a Fast Antiobiotic Susceptibility Test Based on Raman Spectroscopy

Lennard Wendlinger: Establishment of a Rapid Concentration Method for Legionella Pneumophila using MAF-DEAE

Julian Weng: Combination of Solid Phase Extraction and Microarray-based Immunoassays for the Screening of Sulfonamides in Water Samples

Lilly Zacherl: Raman Analysis of Iron-containing Proteins

Richard Zell: Development of Relative Quantitative and Quantitative Approache for the Analysis of Flavouring Substances in Saffron (crocus sativus)

Institute Colloquia

Prof. Dr. Kerstin Leopold, Institut für Analytische und Bioanalytische Chemie, Universität Ulm: Trace Metal Analysis in Environmental Samples - About Picograms and Nanoparticles (19.01.2018)

Dr. Ali K. Yetisen, Havard-MIT Division of Health Science and Technology, Cambridge: Photonic Hydrogel Sensors (19.03.2018)

Prof. Dr. Jürgen Hauer, Professur für Dynamische Spektroskopien, Technische Universität München: Ultrafast 2D Electronic Spectroscopy on Light Harvesting Systems (18.05.2018)

Prof. Dr. Hanno Steen, Harvard Medical School – Boston Children’s Hospital, Department of Pathology: Clinical Proteomics for the Discovery of Diagnostic and Therapeutic Targets - From Monitoring the Health Status of Preemies to Tackling Neurodegeneration in the Elderly (13.07.2018)

Prof. Dr. Joel Pedersen, University of Wisconsin – Madison, Department of Soil Science: Nanoparticle Interactions at Biological Interfaces: Insights from Model Systems (17.07.2018)

Prof. Dr. Janina Kneipp, Humboldt-Universität zu Berlin, Department of Chemistry: Analytical Applications of One- and Two-Photon Excited SERS (23.07.2018)

Prof. Dr. Oliver Hayden, Heinz Nixdorf-Lehrstuhl für Biomedizinische Elektronik, Department of Electrical and Computer Engineering, TranslaTUM, Campus Klinikum rechts der Isar: In Vitro Diagnostics of Peripheral Blood Cells (27.07.2018)

Assoc. Prof. Dr. Ario de Marco, Lab of Environmental and Life Sciences, University of Nova Gorica, Slovenia: Nanobodies as Convenient Reagents for Multiple Biotechnological Applications (14.09.2018)

Prof. Dr. Stephan A. Sieber, Lehrstuhl für Organische Chemie II, Technische Universität München: Chemical Manipulation of Bacterial Pathogenesis (24.09.2018)

PhD Mats Leifels, Visiting Scientist and RUB-RS Fellow, School of Public Health, University of Alberta, Edmonton, Canada: Interaction Between Human Enteric Viruses and Free-living Amoebae in Natural and Artificial Freshwater Environments (12.10.2018)

Prof. Dr. Fang Wang, Institute of Soil Science, Chinese Academy of Sciences, China: Antimicrobial Resistance in Antarctic and Agricultur (06.11.2018)

Teaching

GIST TUM-Asia

Industrial Chemistry (M.Sc.)

Bioengineering & Bioprocessing; Seidel

Chemical Engineering (B.Sc.)

Biochemical Process Engineering; Seidel

TUM

Chemistry (B.Sc./M.Sc.)

Hydrogeological, Hydrochemical and Environmental Analysis Seminar (Hydrogeologisches, Hydrochemisches und Umweltanalytisches Seminar); Elsner, Baumann, Haisch, Knopp.

Graduate Course in Analytical Chemistry: Lecture in Organic Trace Analysis-Physical and Chemical Separation Methods (Nebenfach Analytische Chemie: Vorlesung Organische Spurenanalytik-Physikalisch-chemische Trennmethoden); Elsner, Seidel, Haisch, Ivleva, Bakkour.

Graduate Course in Analytical Chemistry: Lab in Organic Trace Analysis (Nebenfach Analytische Chemie: Kurpraktikum Organische Spurenanalytik); Elsner, Seidel, Haisch, Ivleva, Bakkour

Graduate Course in Analytical Chemistry: Research Lab in Organic Trace Analysis (Nebenfach Analytische Chemie: Forschungspraktikum Organische Spurenanalytik); Elsner, Seidel, Haisch, Ivleva, Bakkour

Trace Analysis Techniques (Spurenanalytische Techniken); Elsner, Seidel, Haisch

Environmental Organic Chemistry: Elsner, Bakkour

Biochemistry and Molecular Biotechnology (B.Sc.)

Biochemical Analytics – Immunoassays and Chiptechnology; Seidel

Biochemistry (B.Sc.)

Trace Analysis for Biochemist; Seide

Geosciences (B.Sc./M.Sc.)

Analytical Chemistry I: Instrumental Analysis for Geoscientists (Analytische Chemie I: Instrumentelle Analytik für Geowissenschaftler); Elsner

Analytical Chemistry II – Organic Trace Analysis for Geoscientists (Chemische Analytik II – Organische Spurenanalytik für Geowissenschaftler); Elsner

Contaminant Hydrogeology (Transport von Schadstoffen im Grundwasser); Baumann

Remediation Design (Erkundung und Sanierung von Grundwasser-schadensfällen); Baumann

Technical Hydrogeology (Technische Hydrogeologie); Baumann

Fluidflow in Porous Media Lab (Hydrogelogisches Laborpraktikum); Baumann, Haisch

Hydrogeochemical Modelling (Hydrogelogische Modelierung II); Baumann

Hydrogeological Field Lab (Hydrogeologische Feldmethoden); Baumann

Hydrogeological Mapping (Hydrogeologische Kartierung); Baumann

Hydrogeological and Hydrochemical Field Trips (Hydrogeologische und Hydrochemische Exkursion); Baumann

Water Chemistry I (Wasserchemie I); Elsner

Water Chemistry II – Hydrocolloids, Micellar Systems and Photochemical Transformations (Wasserchemie II – Hydrokolloide, micellare Systeme und photochemische Umsetzung); Elsner

Hydrochemical Lab (Hydrochemisches Praktikum); Haisch, Baumann

Geothermics/Geoenergy (MSc.)

Hydrochemistry, Corrosion, and Scalings (Hydrochemie, Korrosion und Scalings), Baumann

Equipment

Hydrogeology

Two pilot scale tanks with flow lengths of up to 10 m allow transport experiments in a controlled environment while preserving almost natural conditions. Apart from studies on the transport behaviour of contaminants and colloids, these facilities are used for testing sensor prototypes and serve as a test bed for numerical models

Großhadern Unsaturated Zone field laboratory (10 m deep)

1 Analytical Autoclave, Büchi Midiclave

Dioxin Laboratory

3 High security labs with locks, separate activated carbon filter and high-performance particle filter systems

Aerosol Research

1 Aerosol chamber (1 m3)

1 Aerosol flow tube (10 L)

1 Ozone analyzer (UV absorption)

1 NO/NO_2

analyser (Chemiluminescence)

2 Aerodynamic particle sizers (0.5-25 µm)

1 Berner impactor (9 stages, 50 nm - 16 µm)

1 Electrical low-pressure impactor (12 stages, 30 nm – 10 µm)

2 Low-Volume filter samplers (PM 10, PM2.5)

1 High-Volume filter sampler (PM 2.5)

2 Differential mobility particle sizer systems (10-1000 nm)

2 Diffusion batteries (5-300 nm)

5 Condensation nucleus counters

3 Electrostatic classifiers (10-1000 nm)

2 Spark-discharge soot aerosol generators (polydisperse ultrafine carbon aerosol)

1 Berglund-Liu aerosol generator (monodisperse aerosols, 0.8-50 µm)

1 Floating bed aerosol generator (powder dispersion)

1 Rotating brush aerosol generator (powder dispersion)

1 Tube furnace

1 Cyclone Impinger (Coriolis µ, Berlin)

1 Micro soot sensor with dilution unit

Bioseparation

1 Crossflow-ultrafiltration unit (6 m^2 hollow fibre module, Inge-AG)

1 Munich Microorganism Concentrator (MMC 3)

1 Monolithic Affinity Filtration Unit

Microarray Technology

2 Chemiluminescence Microarray Reader (Immunomat, IWC)

4 Chemiluminescence Microarray Reader (MCR 3, GWK GmbH)

1 Ink-Jet Microdispenser (SciFlexarrayer 31, scienion)

2 Contact Microarrayer (BioOdyssee Caligrapher, BioRad)

1 Cutting Plotter (Graphtec CE6000-40)

Microbiology

1 Flow Cytometer (Cell Lab Quanta SC, Beckman Coulter)

1 Flow Cytometer (CyFlow Cube 6, Sysmex Partec GmbH)

1 Water Microbiology (Colilert-18 and Quanti-Tray 2000, IDEXX)

3 Clean benches

1 Microbiological Incubator (BD 53, Binder)

1 Autoclave (Century 2100, Prestige Medical)

1 Autoclave (SHP Steriltechnik)

1 Bio-2-Aerosol Chamber

1 Level 2 Biosafety laboratory for working with pathogenic bacteria, viruses and molds

Bioanalytics

1 Real-Time PCR (Lightcycler 384, Roche)

1 PCR Safety Cabinet

1 SPR-Biosensor (Biacore, GE)

1 MiCsMAP system (IGGSE) Flow-based Microrreactor & miniNMR

Standard Lab Equipment

1 Lyophilizer (Alpha 1-4 LSC, Christ)

1 Washer Disinfector (DS 500 Lab, International Steel CO.SPA)

1 Ultrapure Water System (Direct-Q 3 UV, Millipore)

1 Refrigerated Centrifuge (Universal 320R, Hettich)

1 Centrifuge (Eppendorf 5804 R)

1 Climatic chamber (Memmert HCP 108)

2 Fluorescence reader systems, time-resolving

3 Photometric reader systems

1 384-channel washer, Biotek

1 Turbidometer (WTW GmbH)

1 Nanophotometer (Implen GmbH)

Chromatography and Particle Separation

3 GCs with FID, NPD, ECD, TEA, and AED

1 Orbitrap-based benchtop MS, Exactive/HCD-System, Thermo Fischer

1 GC/MS, VG Autospec

1 GC/MS, Shimadzu

1 Portable Micro-GC, MITEC

1 Asymmetrical Field-flow-fractionation system, Postnova

2 Concentrators for dynamic headspace analysis

4 HPLC, UV/VIS array detector, programmable fluorescence detector

1 Capillary electrophoresis system

1 Ion chromatograph, Dionex 4500 i

1 Ion chromatograph, Dionex BioLC (Photodiode Array Detector, Electrochemical Detector)

1 Ion chromatograph, Metrohm 881

1 LC system, ECONO

1 Preparative HPLC

1 Zetaphoremeter, SEPHY

Elemental Analysis

1 TXRF, Atomika EXTRA II a

1 Flame-Photometer, Eppendorf ELEX 6361

2 AAS systems with flame atomization, electrothermal atomization, hydrid system, Perkin-Elmer PE 3300, ELAN 4100

1 ICP-MS, Perkin -Elmer Nexion 350D

Laser

2 He/Ne-laser

5 Nd-YAG -laser, pulsed

1 Nd-YAG Laser 2 W cw, 532 nm narrow band

3 Nd-YAG-laser, cw

1 CO_2-laser

3 Dye-laser (tunable with frequency doubler)

5 N_2-laser

8 Diode-lasers (600-1670 nm; up to 2 W CW)

1 Laser diode array with 10 diodes (0.8 µm-1.8 µm)

1 Laser diode with external resonator

2 Optical parameter oscillator (410 nm-2.1 µm)

Optoelectronics/Spectrometer

1 Rowland spectrometer

2 Echelle spectrometer

1 ICCD spectrometer system

1 FTIR-Spectrometer, Thermo Scientific Nicolet 6700

1 Fluorescence spectrometer, Perkin Elmer LS-50

1 Fluorescence spectrometer, Shimadzu RF 540

1 UV/VIS spectrometer, Beckman DU 650

1 UV/VIS spectrometer, analytic jena Specord 250 plus

1 UV/VIS spectrometer, analytic jena Spekol 1500

2 Boxcar integrator

4 Digital storage oscilloscopes (400 MHz, 500 MHz)

3 optical multichannel analysators with monochromators, time-resolving

1 Wavemeter

SEM/Microscopy

1 SEM/EDX system, Zeiss Gemini

1 Polarisation microscope for phase analysis

1 Fluorescence microscope

1 Image analysis software for anutomated image processing

1 Inert gas glovebox

1 Laminar flow box

Raman-Microscopy

2 Laser Raman microscope, WITec alpha300R (532/633 nm)

1 Laser Raman microscope, Renishaw 2000 (514/633/785 nm)

1 Laser Raman microscope, Horiba LabRam HR (532/633/785 nm)

1 Temperature controlled stage (-196 °C – 600 °C, Linkam THMS 600)

Sum Parameters

2 Coulostat for C quantification, Coulomat 702

1 DOC analysator, UNOR 6 N

1 TOC analysator, TOCOR 2

1 AOX/TOX, Sigma

Staff 2018

Director of Institute and Chair

Univ.-Prof. Dr. Martin Elsner

Senior Researchers

Dr. Rani Bakkour
PD Dr. Thomas Baumann
Prof. Dr. Christoph Haisch
Dr. Natalia P. Ivleva
PD Dr. Michael Seidel

Post Docs

Dr. Benjamin Heckel (1/18-12/18)
Dr. Genny Pang (-10/18)
Dr. Gabriel Sigmund (2/18-12/18)
Dr. Klemens Thaler
Dr. Martina Ueckert
Dr. Noemi Utry

Technical & Administrative Staff

Birgit Apel
Christine Beese
Roland Hoppe
Joachim Langer
Susanne Mahler
Cornelia Popp
Hatice Poyraz
Christine Sternkopf
Sebastian Wiesemann

PhD Students

MSc Phys. Emilio Ambra (6/18-)
MSc Wasserb. Sayed Amininejad (-9/18)
MSc Chem. Philipp Anger
MSc Chem. David Bauer
MSc Chem.-Ing. Jonas Bemetz (-5/18)
MSc Chem. Elisabeth von der Esch
MSc Umwelt-Ing. Lorenza Gilardi (4/18-)
MSc Umweltchem. Lisa Göpfert
Exam. Lebensm. Chem. Carolin Hartmann
MSc Chem. Catharina Kober (-12/18)
MSc Erdw. Bernhard Köhl (-6/18)
Dipl.-Phys. Peter Menzenbach
MSc Chem. Verena Meyer
Dipl.-Biochem. Oleksii Morgaienko
MSc Chem. Li Qiu
MSc Chem. Alexander Rinkenburger (-7/18)
MSc Bio. Chem. Sandra Schäfer (-2/18)

MSc Chem. Christian Schwaferts
MSc Biol. Katharina Sollweck (2/18-)
MSc Chem. Yanwei Wang (7/18-)
MSc Chem. Ruben Weiß
MSc Chem. Carina Wismeth (-12/18)
MSc MBT Katharina Zirngibl (ehem. Stutzer)

External PhD Students

MSc Chem. Jessica Beyerl (LMU-Tropeninstitut) (11/18-)
MSc Chem. Matthias Edelmann (TUM, Lebensmittelchem. u. molekulare Sensorik)
MSc Chem. Benno Ehrl (Helmholtz Zentrum München) (-2/18)
MSc Toxikologie Anne Landmesser
MSc Bio. Christina Lihl (Helmholtz Zentrum München)
MSc Biochem. Stefanie Mak
MSc Toxikologie Aileen Melsbach (Helmholtz Zentrum München)
MSc Chem. Janine Potreck (Klinikum rechts der Isar) (2/18-)
MSc Geol. Marina Spona-Friedl (Helmholtz Zentrum München)
MSc Hydrogeol. Fengchao Sun (Helmholtz Zentrum München)
MSc Biochem.Ruoyu Sun (Klinikum rechts der Isar) (-4/18)

Master Students

BSc Biochem. Elisabeth Ackermann (11/18-)
BSc Chem. Franziska Adler (4/18-9/18)
BSc Chem. Matthias Bauer (11/18-)
BSc Chem. Jessica Beyerl (-2.18)
BSc Chem. Christian Biermaier (3/18-9/18)
BSc Ind. Chem. Jorge Adrian Guajardo (TUM Asia) (10/18-)
BSc Ind. Chem. Manjiang Hong (TUM Asia) (-4/18)
BSc Chem. Merlin Junk (9/18-)
BSc Chem. Julia Neumair (4/18-10/18)
BSc Pharm. Elmedina Shimaj (Erasmus) (10/18-)
BSc Daniel Toller (9/18-)
BSc Chem. Markus Weber (6/18-12/18)

Bachelor Students

Nur Aisha Abdul Aziz (-2/18)
Rilette Bautista (-2/18)
Wei Yuan Goh (-2/18)
Sonja Hoffmann (3/18-5/18)
Benedict Horn (3/18-5/18)
Ju Rui Len (12/18-)
Felix Ludwig (4/18-6/18)
Maximilian Maier (9/18-11/18)
Henrdrik Pfaadt (12/18-)
Michael Sandholzer (5/18-7/18)
Sarah Schneidemann (6/18-8/18)
Antonia Seitz (3/18-5/18)
Lennard Wendlinger (4/18-7/18)
Julian Weng (3/18-6/18)
Richard Zell (3/18-5/18)

Guests

MSc Sayed Amininejad (10/18-)
MSc Jonas Bemetz (6/18-)
MSc Bernhard Köhl (7/18)
Dr. Anna Cathrine Neumann PhD
Dr. Genny Pang (11/18-)
Christoph Sauerer (-12/18)
Dr. Jan-Christoph Wolf
Dr. Klaus Wutz

Student Assistants

Elisabeth Ackermann (2/18-9/18)
Ayesha Navaid Anwar (10/18-)
Jessica Beyerl (8/18-9/18)
Christina Glaubitz (3/18-7/18)
Markus Heindl (-2/18)
Alexander Kohles (8/18-)
Leonhard Prechtl (-2/18)
Yasmin Selic (2/18-3/18)
Christopher Wabnitz (6/18-8/18