Institute of Water Chemistry
School of Natural Sciences
Technical University of Munich

Annual Report 2021

Institute of Water Chemistry &

Chair of Analytical Chemistry and Water Chemistry

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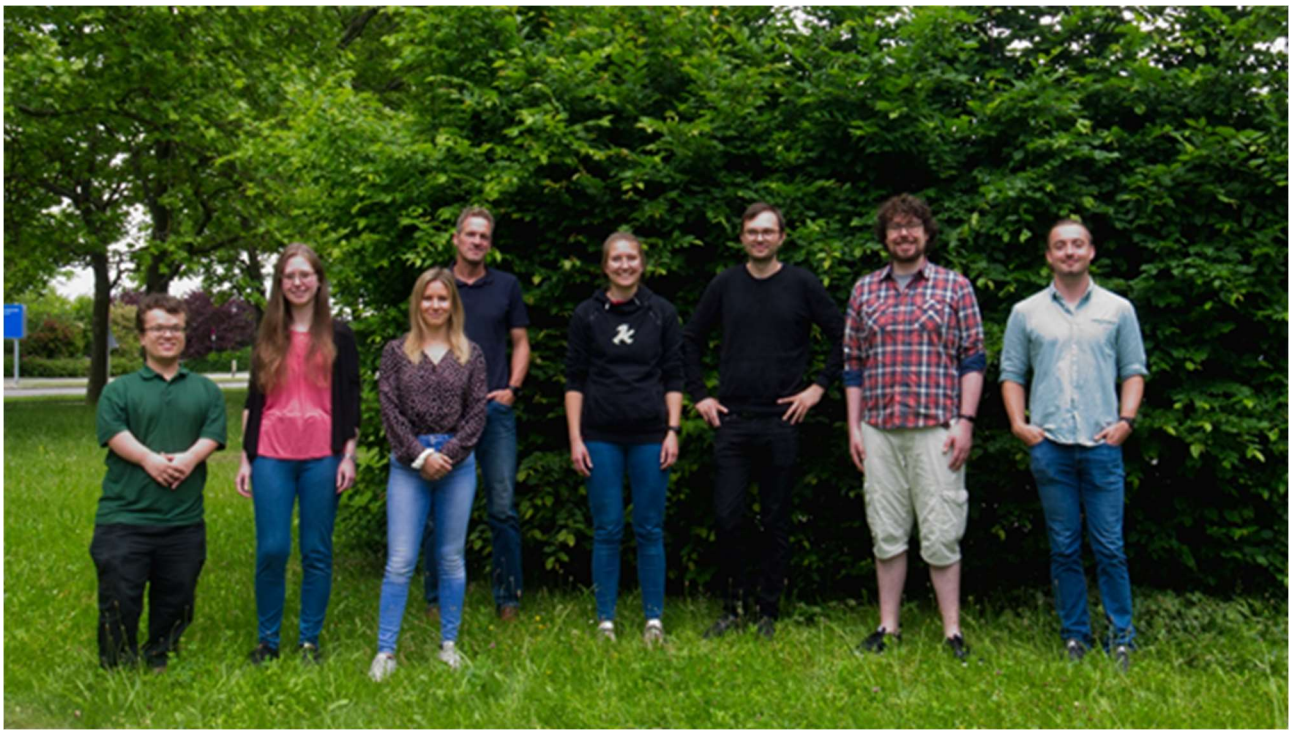
Group photo of the Chair of Analytical Chemistry and Water Chemistry &

Institute of Water Chemistry (IWC) in Raitenhaslach in September 2022



Group photo of the Haisch Group Lasers & Microparticles somewhere in June 2022

Content

Dear colleagues and friends,

it has been our technicians, secretaries and Ph.D. students who have been the pillars of our institute in 2021. Without them, the Herculean task of moving from Großhadern to Garching would not have been possible. Even under adversary circumstances our secretaries Conny and Christine were great in making the best of every situation. Our technicians, in particular Susi and Christine, provided their unwavering support until the last day in Großhadern, while Marco and Felix were at the forefront of accommodating everything in Garching. The Bakkour group had already done the pioneering of setting up much infrastructure in Garching so that moving in was facilitated for the other groups. And then there was the overwhelming support by all Ph.D. students who came to Großhadern in December to help the Haisch group when they were the last to leave the institute building and had to shoulder the greatest burden. In these challenging times we have stayed together as an institute.

An era was coming to a close with the machine shop in Großhadern. Over decades, Sebastian and Roland had been playing not only a supportive, but often rather a pioneering role in the Institute's research. They have designed devices, built prototypes and demonstrators, of which the Munich particle separator even made it into the Deutsche Museum. We do not know how to thank them for everything they have contributed, enabled and designed. Even when they had the invidious task to deconstruct their excellent machine shop in Großhadern, they were helping until the end. A great thank you!

The new year has seen a fresh start in Garching - new labs, new offices and our instruments getting up to pace again. Sonja Rottler has joined us as new secretary, colleagues from the chemistry department are next door now, new students arrive in our labs, and as Corona restrictions are being lifted, the dynamics of institute life is unfolding again. Visit us: our offices are in the red-brown tower of the chemistry building (CH6), third floor, north wing, and our labs in the green tower (CH2), third floor!

There you will find the Seidel group with everything set up for research on Bioanalytics and Microanalytical Systems. The laboratories include facilities for microarray production, synthesis of magnetic nanoparticles, ELISA implementation, or MCR measurements of micropollutants such as pharmaceuticals and toxins. In addition, an expert Bio2-laboratory enables research on pathogens and antibiotic-resistant bacteria with quantitative culture-independent methods (nucleic acid amplification tests or immunoassays) on real water samples. A special feature is the bioaerosol chamber, in which the LegioRapid project develops standardized sampling protocols for pathogens such as *Legionella pneumophila* from air.

Next door are our labs for water chemistry, organic synthesis, as well as analysis of inorganic and organic chemical water components. The green tower (CH2) harbors our liquid- and gas chromatography-based routine analysis together with no less than three specialized isotope ratio mass spectrometers, whereas the yellow tower (CH3), fourth floor hosts our analysis of inorganic water constituents, among others, ICP-MS, ion chromatography and flame photometry. In these labs, the Bakkour group is developing innovative sampling and clean-up methods for sensitive isotope analysis of organic micropollutants, while the Elsner group is advancing applications of compound-specific isotope analysis to trace pollutant sources and their transformation in the environment.

Again next door in CH2, you find the Ivleva group with their focus on dedicated particle analysis. This research is supported by three Raman microspectroscopy instruments, a raster electron microscope, a clean bench for sample preparation and field-flow-fractionation for particle separation. The stage is set for the prime goals of the Raman/REM group: advancing nanoplastics analysis, as well as studying plastics biodegradation by a combination of Raman microspectroscopy and stable isotope labelling. Within this fruitful research direction, particular highlights of last year were the PhD thesis of Elizabeth von der Esch, who defended with “summa cum laude”, as well as an invited review of Natascha Ivleva in Chemical Reviews. Contgratulations, Eli and Natascha!

The Haisch group was the last to leave Großhadern and is still waiting to move into the new rooms in Garching, but has nonetheless been as successful as ever. Raman microscopy was applied also here for variety of topics, ranging from the investigation of inorganic material over microbiological questions to investigations in art history in international collaboration. Among others, application of Raman spectroscopy for process monitoring was intensified with colleagues next door from TUM and LMU. Another focus was set on fundamental as well as applied research on atmospheric ionization mass spectrometry, using the SICRIT ionization source from our friends from Plasmion GmbH.

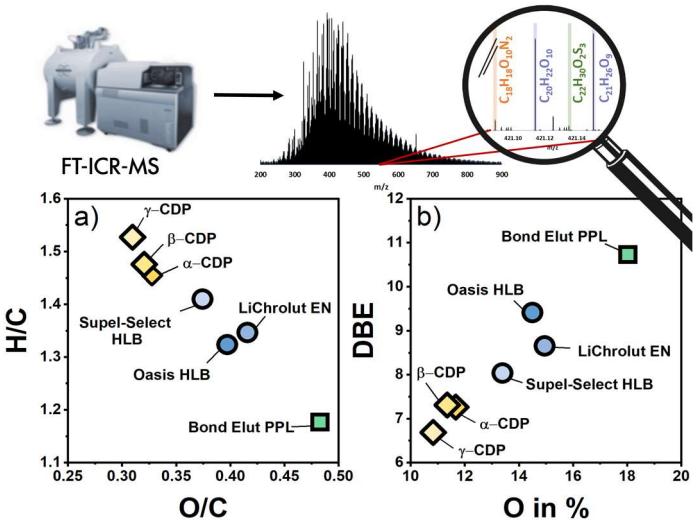
In conclusion, I take the opportunity again to thank to all members of our institute - Ph.D. students, technicians, secretaries, Postdocs and guest scientists - for their dedication, positive attitude and resistance to frustration over the last year. And of course to you, our friends – for your continued support! Come and visit us in our new home in Garching!

Kind regards,

Selectivity of Solid Phase Extraction Sorbents Traced by Ultrahigh-Resolution FT-ICR Mass Spectrometry

Molecular analysis of dissolved organic matter (DOM) in SPE extracts can elucidate sorbent selectivity and thus contribute to optimized sample preparation procedures for matrix susceptible analytics.

State of the Art Analytical techniques that are susceptible to matrix effects, such as quantitative LC-MS or sensitive compound-specific isotope analysis (CSIA), demand selective sorbent materials for analyte enrichment prior to analysis. Recently, we demonstrated the benefit of superior selectivity of cyclodextrin-based (CDP)[1] over conventional solid phase extraction (SPE) sorbents for CSIA of micropollutants[2]: stronger discrimination against DOM reduced matrix loads in CDP extracts enabling up to six times lower method quantification limits of CSIA. Knowledge about underlying causes is warranted to further optimize selective sample preparation.



a) Average H/C- and O/C-ratios, and b) average double bond equivalents (DBE) as function of oxygen contents of DOM-extracts after SPE of surface water using cyclodextrin polymers (yellow), conventional sorbents (blue), and Bond Elut PPL (green).

Analytical Approach To elucidate sorbent selectivity on the molecular level, we characterized and compared DOM compositions in extracts from surface water when using CDPs of different cavity size (α-, β-, γ-CDP) and conventional polymeric SPE sorbents (Oasis HLB, LiChrolut EN, Supel-Select HLB) under otherwise identical conditions (pH = 7, methanol elution). Analysis was performed by ultrahigh-resolution Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) and molecular formula assignment was performed using an in-house written software tool.

Results DOM characterization in extracts revealed sorbent selectivity driven by molecular properties of matrix compounds (i.e., polarity and aromaticity). In comparison to Bond Elut PPL extracts, which yield spectra that reflect intrinsic DOM diversity,[3] CDPs discriminated more strongly against highly oxygenated (high O/C in Fig. 1a, high %O in Fig. 1b), as well as unsaturated, aromatic compounds (low H/C in Fig. 1a, high DBE in Fig. 1b) than conventional SPE sorbents. Our results highlight the importance of diligently chosen extraction materials for analytical applications when matrix effects are expected. Insights into DOM composition of extracts can further aid in tailoring advanced clean-up strategies to remove remaining organic matrix.

David Glöckler, Rani Bakkour

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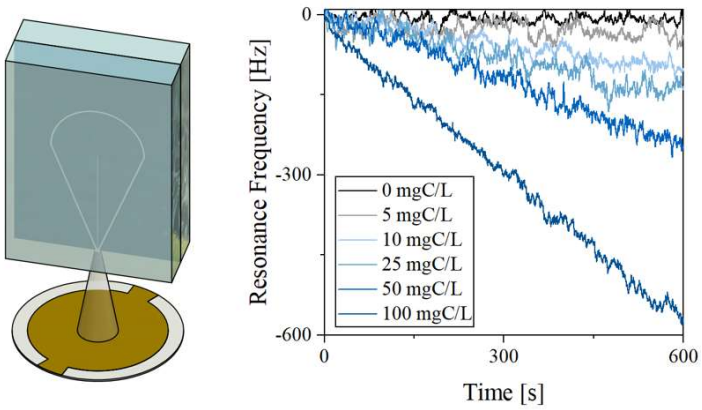
Cooperation
Prof. Dr. Philippe Schmitt-Kopplin & Dr. Mourad Harir
Helmholtz Zentrum München

Gravimetric Quantification of dissolved Natural Organic Matter using a Quartz Crystal Microbalance

Dry mass sensing using a quartz crystal microbalance and a microfluidic spray-dryer is promising for the online monitoring and quantification of matrix compounds in organic extracts during purification.



Left side: Scheme of the microfluidic spray-dryer for deposition of NOM solutions onto a QCM sensor chip. Right side: Gravimetric detection of aqueous NOM solutions using the microfluidic spray-dryer. Spray-drying of different concentrated NOM solutions leads to a linear decrease of the measured resonance frequency with time. The slope is dependent on the concentration.

State of the Art Accurate isotope measurements in compound-specific isotope analysis (CSIA) are often only possible after extensive purification of the sample.[1] Automating the purification and its optimization can reduce workload and analysis time significantly. To this end, both the target compounds and the interfering matrix need to be monitored online and quantified. While methods for online analyte detection are typically in place, matrix monitoring poses a bigger challenge. A sensor that can potentially solve this problem is the Quartz Crystal Microbalance (QCM).

Analytical Approach Recently, dry mass sensing using a QCM was used to detect proteins online after liquid chromatography. To this end, a small part of the eluate was deposited on the QCM using a microfluidic spray-dryer.[2] In this work, we explore the feasibility of combining a QCM with a spray-dryer to online monitor and quantify natural organic matter (NOM) in the purification of organic extracts.

Results Spraying aqueous NOM solutions onto the QCM lead to a linear decrease of the measured resonance frequency with time. There is a linear correlation between the sprayed NOM concentration and the resonance frequency decrease (coefficient of determination R^2 of 0.998). The limit of detection was 18 mg/L, which is equal to a sprayed mass of 45 ng/min. This sensitivity is sufficient for the online detection of NOM in organic extracts in CSIA sample preparation. Settings were additionally optimized to measure water, acetonitrile, and methanol mixtures, which is possible with a spraying height of 3 cm, a flow rate of 150 µL/h and a pressure of 2.5 bar. Our findings illustrate that dry mass sensing using a QCM is promising for the online detection of NOM during the purification of organic extracts.

Christopher Wabnitz, Aoife Canavan, Rani Bakkour

Funding
IWC-TUM

Cooperation
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University of Cambridge

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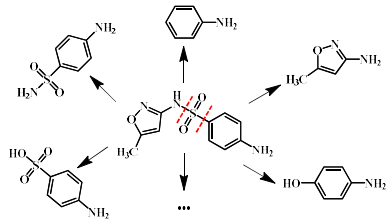
Metabolic Mechanism of Sulfonamide Cleavage: A Combined Computational and Experimental Study on Sufamethoxazole

Quantum chemical calculations can help decipher the metabolic mechanisms of micropollutant degradation in the environment by predicting isotope effects in comparison with experimental observations.

State of the Art In recent years, antibiotics have drawn great attention because of their potential to generate antibiotic resistance.[1] To understand enzymatic degradation of these micropollutants, computational chemistry approaches such as quantum chemical calculations can compute electronic structures for enzymatic models with hundreds of atoms. Such characterizations are able to predict intermediates and transition states during metabolic reactions from both structural and energetics aspects.[2] They, therefore, represent a powerful tool to understand detailed metabolic mechanisms, and to predict associated isotope effects. Comparison with experimental values can elucidate biochemical transformations to aid in understanding antibiotic resistance, and in developing potent enzymes to curb micropollutant contamination.



Substrate	SMX (neutral)	SMX (protonated)	SMX (unprotonated
SMX	-1174.536958	-1174.874446	-1173.984726
radical aniline	-286.5334552	-286.8769033	-286.5334552
radical sulfonamide	-887.8669036	-887.8669036	-887.3294544
BDE C-S	**85.72**	**81.98**	**76.44**
radical_anilineSO2	-834.8307684	-835.1555596	-834.8307684
radical_Nitrogen_isoxazole	-339.6191804	-339.6191804	-338.9935838
BDE S-N	**54.60**	**62.57**	**100.64**

The possible metabolites of SMX (the top). The C-S and N-S bond dissociation energies of neutral SMX, protonated SMX and deprotonated SMX (the bottom).

Analytical Approach Quantum chemical calculations by QRCA 4.2.1 software are being conducted to explore putative metabolic mechanisms, and to screen for possible reaction pathways and metabolites.

Results In this study, sufamethoxazole (SMX) was selected as a model antibiotic substrate, since it is widely used in veterinary and human medicine[1]. From the preliminary computed bond dissociation energies (BDE), the S-N bond of SMX is more easily broken than the C-S bond. In addition, compared with the protonated SMX and deprotonated SMX, the cleavage of S-N bond of neutral SMX has the smallest BDE, suggesting that it may be the most dominant pathway.

Lihong Chai

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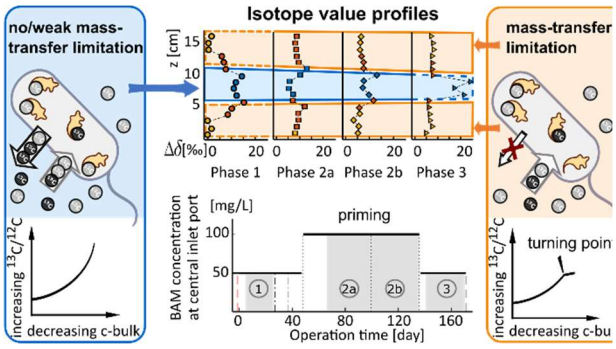
Dr Etienne Derat (Sorbonne Université)

Prof Lynn Kamerlin (Uppsala University)

Prof José Manuel Sanchez Ruiz (University of Granada)

Towards improved bioremediation strategies: Response of BAM-degradation activity to concentration and flow changes in an inoculated bench-scale sediment tank

Isotope fractionation profiles identify putative bottlenecks of organic trace contaminant degradation in a sediment tank and suggest the application of priming as promising bioremediation approach in biofilters.



Long term monitoring of concentrations, as well as carbon and nitrogen isotope values of BAM in a bench-scale sediment tank revealed limitations of biodegradation in the long-term performance of a sediment biofilter. While isotope profiles indicate that biodegradation activity became *partially* rate-limiting at low concentrations, they show that mass transfer never became *completely* rate-limiting in the long run implying that bacterial adaptation decreased at low concentrations and needed periodic re-stimulation for optimum performance.

State of the Art Compound-specific isotope analysis (CSIA) can reveal mass-transfer limitations during biodegradation of organic pollutants by enabling the detection of masked isotope fractionation.[1, 2] Here, we applied CSIA to monitor the adaptive response of bacterial degradation in inoculated sediment to low contaminant concentrations over time.

Analytical Approach We characterized *Aminobacter* sp. MSH1 activity in a flow-through sediment tank in response to a transient supply of elevated 2,6-dichlorobenzamide (BAM) concentrations as a priming strategy and took advantage of an inadvertent intermittence to investigate the effect of short-term flow fluctuations in long-term performance.

Results Priming and flow fluctuations yielded improved biodegradation performance and increased biodegradation capacity, as evaluated from bacterial activity and residual concentration time series. However, changes in isotope ratios in space and over time evidenced that mass transfer became increasingly limiting for degradation of BAM at low concentrations under such stimulated conditions in the long run, and that activity decreased further due to bacterial adaptation at low BAM (µg/L) levels. Isotope ratios, in conjunction with residual substrate concentrations, therefore helped identifying underlying limitations of biodegradation in such a stimulated system, offering important insight for future optimization of remediation schemes.

Fengchao Sun

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Cooperation

Prof Olaf Cirpka

Prof. Christian Griebler

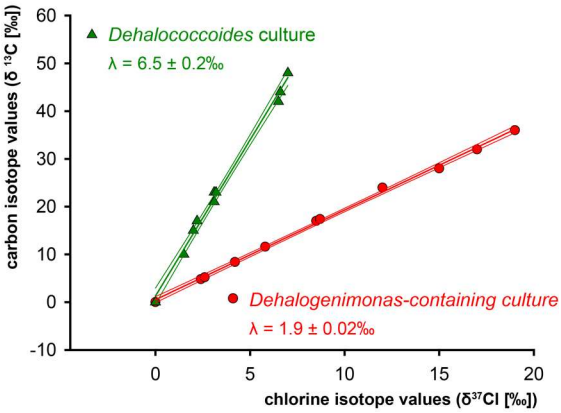
Dr. Martin Thullner

Mechanistic Basis of Biotic Chlorinated Alkane Reduction: Evidence of Nucleophilic Substitution (S_N2) with Vitamin B_{12}

Nucleophilic (S_N2) attack of cobalamin is found to lie at the heart of biotic chlorinated alkane reduction, providing an important cue to understanding metabolite formation in bioremediation.

State of the Art Chlorinated alkanes are notorious groundwater contaminants. Their natural reductive dechlorination by microorganisms involves reductive dehalogenases (RDases) containing cobamide as a cofactor. Underlying mechanisms of reductive dehalogenation, however, have remained uncertain.

Analytical Approach Here, observed products, radical trap experiments, UV-Vis and mass spectra demonstrate that (i) reduction by cobalamin (Vitamin B_{12}) involved chloroalkyl-cobalamin complexes (ii) whose formation involved a second order nucleophilic substitution (S_N2). Dual element isotope analysis subsequently linked insights from our model system to microbial reductive dehalogenation.



1,2-Dichloroethane (1,2-DCA) dehalogenation by *Dehalococcoides* and *Dehalogenimonas* cultures showed distinctly different dual element (carbon / chlorine) isotope effect trends.(1) Here we show that the trend with *Dehalococcoides* matched that with vitamin B_{12} where a second order nucleophilic substitution (S_N2) involved chloroalkyl-cobalamin complexes, as revealed by observed products, radical trap experiments, UV-Vis and mass spectra.

Results Identical observed isotope effects in reduction of trichloromethane by *Dehalobacter* CF50[2] and cobalamin indicated the same underlying mechanism, as did identical isotope effects in reduction of 1,2-dichloroethane by *Dehalococcoides*[1] and cobalamin. In contrast, a different, non-S_N2 reaction was evidenced by different isotope effects in reaction of 1,2-dichloroethane with *Dehalogenimonas*[1] illustrating a diversity of biochemical reaction mechanisms manifested even within the same class of enzymes (RDases). This study resolves open questions in our understanding of bacterial reductive dehalogenation and, thereby, provides important information on the biochemistry of bioremediation.

Benjamin Heckel

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Funding

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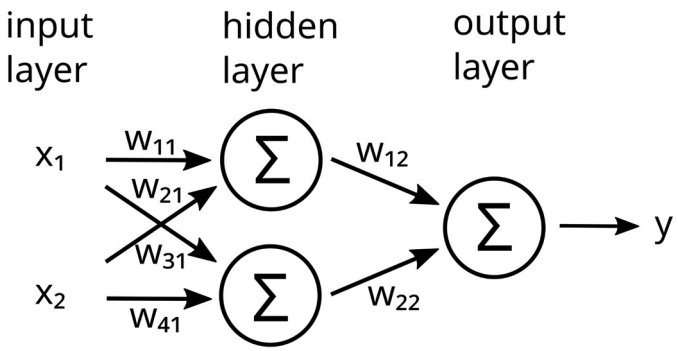
Data Mining for Discovering Environmental Pollution

The large amounts of data created by non-target screening of surface water samples with LC-HRMS/MS require new approaches for effective evaluation and data mining. This project aims to explore the use of machine learning algorithms for processing these measurements.



A diagram of an artificial neural network, which is a machine learning algorithm. Each neuron, represented by a circle, takes the input values x, multiplies them with the corresponding weights w and sums them up. To the sum the activation function is applied, typically f(x) = max(0,x) for hidden layers and f(x) = x for the output layer. The result is then used as the input for the next layer of neurons or in case of the output layer as output y. During the training of the neural network, the weights w get adjusted.

State of the Art Manmade organic compounds are continuously released from urban and agricultural activities into surface waters. Many new chemicals are not yet recognized, not included in monitoring and may even be of unknown structure and of unknown toxicity. Liquid chromatography coupled to high resolution tandem mass spectrometry is currently the main tool for non-target screening of surface water. However, this method produces complex datasets which warrant new ways of processing.

Analytical Approach Due to the increased processing power of modern computers and the development of new toolkits, machine learning has recently found usage in a large variety of fields. One strength of machine learning is pattern recognition in large datasets. We want to exploit this ability to improve the data processing of non-target screening data in different ways.

One aspect is the reduction of the complexity of the dataset by identifying signals in the spectrum which are caused by the same substance. Currently this is mainly done by applying chemical knowledge like adduct formation and the recognition of isotope patters. We want to add a statistical approach by grouping signals by their tendency to always appear together in a large number of measurements.

A second aspect is the prediction of the behavior of a substance in the measurement solely by its structure and its chemical properties. Building on existing approaches like retention time prediction and *in silico* fragmentation we want to create a machine learning model which takes a compound and a measurement and checks if the analyzed sample contains the compound.

Additionally, we want to identify markers for microbiological pollution in the non-target screening spectra. This shall be achieved by training a machine learning model with spectra and the results of microbiological measurements of the same sample and afterwards reverse engineering the model to identify the markers.

Leonhard Prechtl

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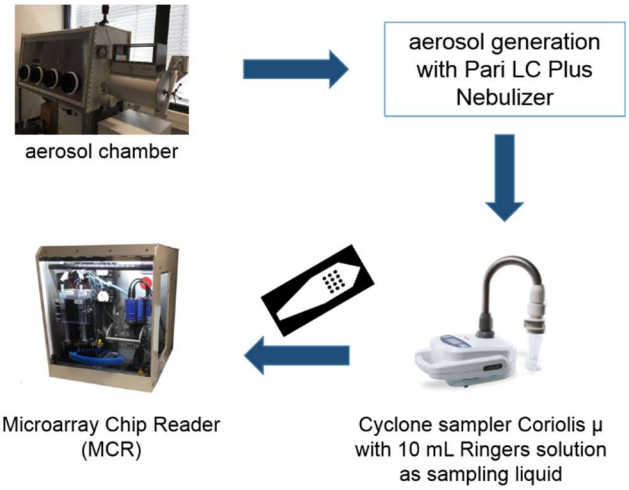
Cooperation
Zweckverband Landeswasserversorgung BW

Development of sampling and quantification strategies for *Legionella pneumophila* in aerosols

Inhaled aerosols of cooling systems, which are contaminated with *Legionella pneumophila,* can cause a severe case of pneumonia. Therefore, it is important to have suitable strategies for sampling and analyses of this pathogen.

State of the Art *Legionella* outbreaks have occurred repeatedly in cooling towers in recent years.[1] So far, the 42. BImSchV only regulates the monitoring of *Legionella pneumophila* concentrations in water, but not in aerosols. In addition, the correlation between the concentration in water and in air has not been fully investigated yet. Together, this motivates further in-depth research on this topic. The problem with the analysis of *L. pneumophila* is that it can enter a viable-but-not-culturable (VBNC) state. To avoid underdetermination and long analysis time through cultivation, it is necessary to develop culture-independent methods.



Schematic workflow for experiments with bioaerosols: generation of aerosols with *L. pneumophila* in aerosol chamber with Pari LC Plus Nebulizer, sampling with cyclone sampler (Coriolis µ) and subsequent performing of a chemiluminescence sandwich microarray immunoassay (CL-SMIA) on a Microarray Chip-Reader Research (MCR-R).

Analytical Approach All experiments with bioaerosols were performed in a bioaerosol chamber[2], so there is no risk of exposure. Preliminary tests to characterize the Coriolis µ were first done with *E. coli* and later with *L. pneumophila* Subtype Bellingham. The quantification took place on different flow cytometers (Sysmex and rqmicro). For the subtyping a chemiluminescence sandwich microarray immunoassay (CL-SMIA) on a Microarray-Chip-Reader (MCR-R) was performed.

Results Before experiments with pathogen bioaerosols were done, the tightness of the aerosol chamber was confirmed by using non-pathogenic *E. coli*. After that, the preliminary tests with *E. coli* showed that the biological sampling efficiency of the Coriolis µ was best with Ringers Solution as sampling liquid and with *L. pneumophila* survival rates up to 90% were determined. The antibody-based CL-SMIA could be performed on an improved MCR-R instrument. For the first time viable *L. pneumophila* Subtype Bellingham was successfully identified after sampling with the Coriolis µ by CL-SMIA.

Lena Heining

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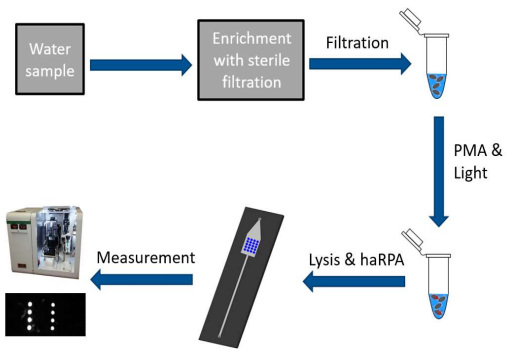
Establishment of a standardized method for molecular biological quantification of *Legionella* in exhaust air purification systems

In the future viable *Legionella* shall be detected fast without the risk of under- or overestimation. Additionally, the differentiation of viable and dead cells shall allow a reliable monitoring to assess the success of clean-up by biocides in all kind of freshwater systems.



Schematic workflow of the integrity haRPA

State of the Art. Due to an increasing number of legionellosis outbreaks in the last years and new guidelines (e.g. 42. BImSchV), the importance of a reliable *Legionella* detection method for, e.g., cooling towers, evaporative cooling systems and air filter systems is becoming more and more important. While the risk in cooling systems is already well understood, risk assessments have not yet been performed for biofilters that are in wide use, e.g. in pig farms. To understand if there is a potential risk for the workers, a rapid culture-independent detection method needs to be developed. Molecular biological methods like qPCR and isothermal nucleic acid amplification methods are able to detect *Legionella spp.* without underestimation and can differ between infectious and dead cells.[1]

Analytical Approach. Extracted *Legionella* spp. DNA from concentrated water samples is amplified by the isothermal heterogeneous asymmetric recombinase polymerase amplification (haRPA) using immobilized primers on a DNA microarray targeting the 16S rRNA Gene. The amplicons can be quantified after a chemiluminescence reaction by visible readout with a CCD camera. To distinguish between viable and dead cells, a DNA-intercalating dye propidium monoazide (PMA) is added. It can pass the cell membrane of dead cells and inhibit the amplification of the haRPA.

Results. The haRPA assay[1] was optimized to increase the sensitivity and a suitable automated DNA-extraction method as well as an enrichment via sterile-filtration was implemented for the analysis of real samples. The sensitivity of the haRPA detection is comparable to the commercial available *Legionella spp.* qPCR detection kit. To further increase the sensitivity, the extraction methods from other kits will be analyzed and compared with the current approach. For the risk assessment of biofilters in pig farms, first samples were taken from the Thünen-Institute and analyzed via culturing, qPCR and haRPA. In the winter period, no *Legionella* spp. were found at 6 sampling sides. Further analyses in the summer period will show if *Legionella* is a potential problem in these filters.

Gerhard Schwaiger

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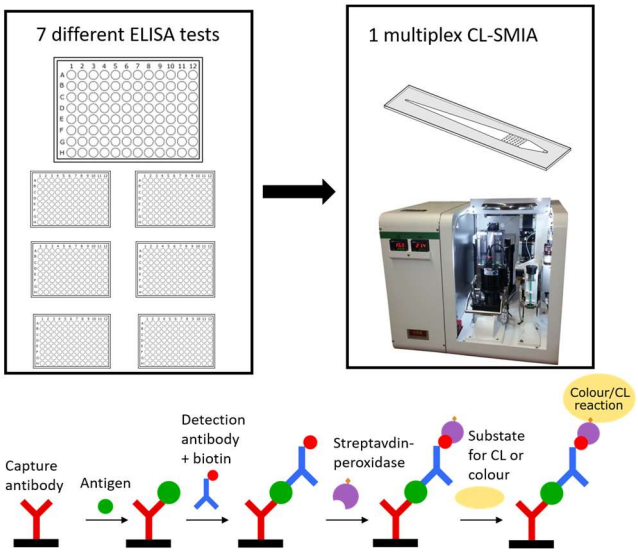
Cooperation
Thünen-Institut für Agrartechnologie

Establishment and analytical characterization of sandwich-ELISAs for the determination of protein biomarkers from nasal secretions

Allergies, bacterial and viral infections, lead to different biomarker compositions in nasal secretions. For seven biomarkers, commercially available sandwich-ELISAs were characterized and established. In a next step, they are applied in a flow-based chemiluminescence sandwich microarray immunoassay (CL-SMIA).

State of the Art Allergies are often misdiagnosed as bacterial infections. The go-to treatment for this type of infections are antibiotics, which, if used excessively, can lead to resistance.[1] Hence, a rapid, cost efficient and time saving method of distinguishing between allergies, bacterial and viral infections is crucial. We want to establish a flow-based CL-SMIA[2] based on commercially available antibody sets used for ELISAs in micro titer plates.



Picture above: Transferring 7 individual ELISA tests to a flow-based multiplex CL-SMIA.

Picture below: Principle of sandwich immunoassay.

Analytical Approach For performing sandwich-ELISAs, the ELISA DuoSets from R&D Systems for human Periostin, IL-29, IL-24, IL-37, Uteroglobin, IFN-β and Eotaxin-3 were used. The assay was optimized in regard to the concentrations of capture and detection antibodies by using grid experiments, as well as different blocking agents. Subsequently, these parameters were transferred to the calibration of the biomarkers.

Results The commercially available antibodies could be optimized in their sensitivity by changing their concentrations – often even to a lower concentration, than stated by the manufacturer. In the calibration experiment, IL-29 and IFN-β showed the best LODs of 1.772 pg/mL and 1.875 pg/mL, respectively. Even so, the overall working ranges were not yet sufficient for the intended use. Hence, in the next step the immunoassay will be established with CL-SMIA on the microarray analysis platform MCR-R. With this approach, we target a more sensitive and rapid detection of the antigens, as well as the implementation of a multiplexing approach.

Marie Kröger, Julia Neumair

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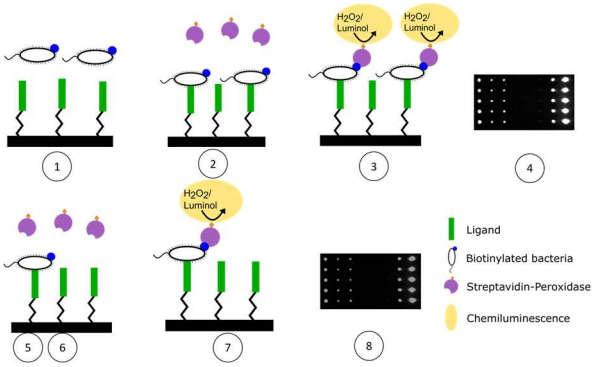
Flow-based chemiluminescence platform for the screening of affinity binders to bacteria

For fast affinity ligand screening, a flow-based chemiluminescence microarray platform was established. Different ligands and elution buffers were investigated for *Escherichia coli* and *Enterococcus faecalis*.

State of the Art During infections of body fluids pathogens often occur in low concentrations. Hence culture-based methods, the current gold standard of detection, are often a critical time limitation in the diagnosis of sepsis. Potentially, the situation could be dramatically improved by monolithic affinity filtration (MAF) for preconcentration.



Workflow of the ligand screening: (1) biotinylated bacteria bind on the ligands, (2) Strep-HRP binds on biotin and (3) catalyzes a CL reaction, (4) which is detected by a CCD camera. Then (5) the bound bacteria are eluted, (6) Strep-HRP binds again and (7) another CL reaction is catalyzed and (8) detected.

Analytical Approach New affinity ligands which bind to pathogens are important for MAF. A flow-based chemiluminescence microarray was used to screen a diverse array of affinity ligands. As surface, a polycarbonate coated with succinylated Jeffamine® ED-2003, a diamino-PEG/PPG triblock copolymer, was used. Affinity ligands were immobilized and the flow-through microarray was assembled. Measurements were carried out on the MCR-R (microarray chip reader – research). Biotinylated bacteria were incubated in a stopped-flow on the chip. After blocking the surface with casein, streptavidin coupled with horseradish peroxidase (Strep-HRP) was used to bind the biotin and to catalyze a chemiluminescence (CL) reaction of luminol and hydrogen peroxide. The signal was recorded by a CCD camera. After this first measurement, elution was performed by flushing the chip with an elution buffer and the chip was measured again, starting from the Strep-HRP step.

Results The assay was performed with biotinylated *E. coli* and *E. faecalis*, which are gram-negative and gram-positive bacteria, respectively. The affinity ligands tested were Polymyxin B (PmB), Concanavalin A, Lysozyme, polyclonal antibody against *E. coli* and polyclonal antibody against *Enterococci*. For elution two different modes were tested: first, the elution buffer was flushed by hand through the chip; second, the buffer was incubated one minute on the chip. For *E. coli*, PmB and the anti- *E. coli* antibody worked best for capturing, where the best elution strategies was use of a 100 mM methyl-α-D-mannopyranoside solution with one-minute incubation and 100 mM glycine at pH 2.5 without incubation, respectively. For *E. faecalis*, the anti-*Enterococci* antibody was the best as well. We could show that a screening platform is important for finding the best combination of affinity ligands and elution buffer as pretest for experiments with MAF.

Julia Neumair

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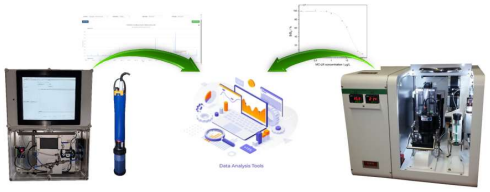
Klinik und Poliklinik II, Klinikum Rechts der Isar (TUM)

Development of an early warning system for increased algal growth and release of algal toxins in surface waters by multiple sensors and online data processing

Currently, hazard assessment is based on experience, visual inspection of water bodies, and discrete sampling. Despite these efforts, accidents continue to occur. For prevention, comprehensive monitoring of potentially endangered waters is urgently needed. Therefore, an online monitoring system with cloud-based automated data processing is warranted.



Communication of the TRITON water sensor system (left) with the MCR-R (right) via an online data management system.

State of the Art Algal blooms are rapid mass proliferations of cyanobacteria. Favored by climate change and eutrophication of water bodies, the phenomenon has become more and more frequent in recent years. An exponential growth spurt of cyanobacteria clouds the water and negatively impacts aquatic macrophytes and living organisms. During algal blooms, the load of cyanotoxins such as microcystin-LR increase in the water, causing adverse effects on the affected ecosystem and posing a threat to human health. ELISA or HPLC-PDA, HPLC-FLD, and LC-MS/MS are the current methods for the quantification of microcystins.[1,2] Analytical microarrays are able to quantify different toxins in parallel.[3] For an early warning system an online approach is needed which measures continuously chemical and physical parameter by a sensor system. Using artificial intelligence, the system is trained for rapid data interpretation if an algae bloom arises. Analytical microarrays are important to confirm the production of cyanotoxins and to correlate their finding with sensor data.

Analytical Approach The TRITON online monitoring system is designed to collect chemical data that can evaluate growth of cyanobacteria online by means of an algorithm and an online data processing system. The physical and chemical sensor system is combined with a biosensor analysis system that determines cyanotoxins such as microcystin, anatoxin or saxitoxin fully automated on the platform MCR-R. A regenerable indirect competitive microarray immunoassay is applied, which can simultaneously quantify different cyanotoxins. In addition, a 3D chip for automated and continuous enrichment by flow-through immunomagnetic separation of cyanotoxins is under development for continuous sampling of surface water.

Andreas Auernhammer

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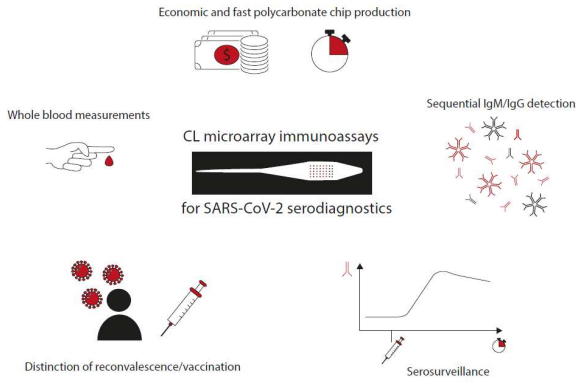
A.U.G. Signals Ltd.
Hydroisotop GmbH

Optimization and extension of a SARS-CoV-2 antibody chemiluminescence microarray immunoassay (CL-MIA) for point-of-care (POC) applications

The COVID-19 pandemic has kept the world in suspense for almost two years now. While it was hoped that vaccinations would pave the way back to normality, we are now facing breakthrough infections that often go unnoticed, making broad serological monitoring with POC methods an important tool in the way out of the pandemic.



Possible point-of-care applications for the SARS-CoV-2 antibody CL-MIA.

State of the Art Over the last two years, more than 5 mio. people died from infection with SARS-CoV-2. As even vaccines do not necessarily protect from infection, serosurveillance is crucial to gain deeper insights in mechanisms of immunity. Typical antibody tests have the drawbacks that they are, among others, time-consuming and laborious. Additionally, most tests cannot distinguish vaccinated and convalescent individuals, making it impossible to detect vaccination breakthroughs.

Analytical Approach We optimized the previously developed CoVRapid CL-MIA[1] for the use of polycarbonate (PC) microarray chips to reduce chip costs, production time, assay time and sample amount. On these chips, different SARS-CoV-2 antigens were immobilized covalently and then used for an indirect non-competitive microarray immunoassay on the novel microarray platform MCR-R. The principle was used for different POC applications, giving serological information in minutes without the need of specialized laboratories or extensive manual steps.

Results The CL-MIA on PC microarray chips achieved a reduction of production time, costs, and sample amount by approx. 90% and of assay time by 50%. Additionally, a diagnostic sensitivity and specificity of 100% was obtained. In terms of POC applications, the use of whole blood was proven possible, as well as the sequential measurement of IgM and IgG, the distinction of vaccinated and convalescent individuals and the semiquantitative progress measurement of antibody titer after vaccination. Therefore, this CL-MIA is a valuable and versatile tool in SARS-CoV-2 serosurveillance, with the potential to contribute towards finding a way out of the pandemic.

Julia Klüpfel

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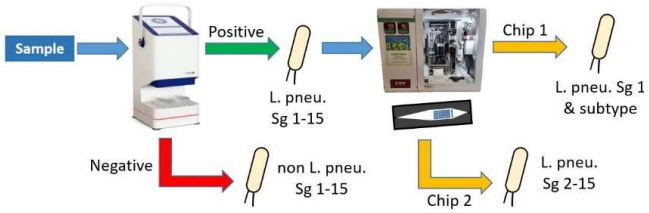
ISAR Bioscience GmbH

Rapid detection of *Legionella pneumophila* in open recooling systems

To confirm the presence of *L. pneumophila* in open recooling systems rapid screening methods are important. The combination of immunomagnetic separation with flow cytometry (IMS-FCM) and the chemiluminescence sandwich microarray immunoassay (CL-SMIA) are two screening assays which can be combined to report the water quality of such systems and determine the species subtype in parallel.

State of the Art According to the 42. BImSchV the gold standard to determine the microbiological exposure of open recooling systems is the culture method. This method needs 7 – 10 days for detection of *Legionella spp.* If the action value of 10,000 *Legionella* spp. / 100 mL is exceeded, a serotyping is recommended.[1] Rapid methods are needed to proof the hygienic treatment process in less than 10 days.



General workflow and data interpretation of the IMS-FCM and CL-SMIA. If a quantitative positive result after IMS-FCM is determined, then the sample contained *L. pneumophila* Sg 1 – 15. Afterwards, the IMS enriched bacteria can be used to perform a CL-SMIA to determine the Sg 1 subtype or Sg 2 - 15.

Analytical Approach, A sample volume of 100 mL was sterile filtered for IMS-FCM. The eluate was incubated with reagents which include a set of antibodies labeled with a dye and antibody-labeled magnetic particles. The IMS and the FCM was performed automatically in the rqmicro.COUNT device which is able to quantify *L. pneumophila Sg 1- 15* within the relevant concentration range according to the 42. BImSchV (100 – 10^5 cells / 100 ml). The IMS-enriched *L. pneumophila* bacteria were collected and after short cultivation in liquid media a CL-SMIA on the LegioTyper was performed for Sg 1 subtyping.[2] In this way highly pathogenic species could be identified in 35 min.

Results Samples from two evaporative systems were investigated after biocide dosage by a combination of IMS-FCM and CL-SMIA. The detected concentrations by IMS-FCM were 9810 ± 661 cells/100 mL and 1922 ± 68 cells/100 mL, respectively. Culture positive was only the sample with higher cell concentrations. The CL-SMIA of this sample showed no significant pattern for any subtype, whereas the polyclonal antibody against *L. pneumophila* indicated a signal that enabled presents of serogroup Sg 2 – 15. With this new method, we could more easier and rapid control the effectiveness of the disinfection process and we could in parallel give information about the found serotype after cultivation.

Philipp Streich

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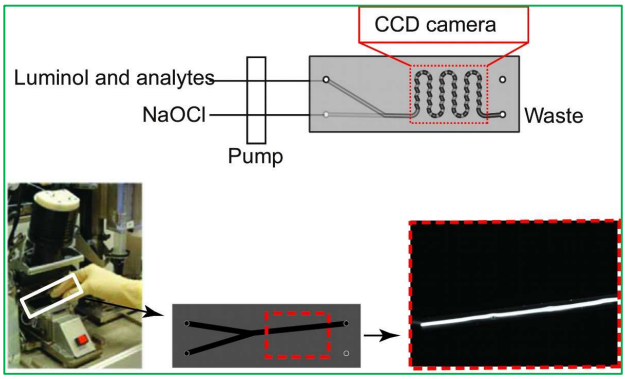
Bavarian Health and Food Safety Authority, Association of German Engineers, GWK Präzisionstechnik GmbH, VDI e.V. Institute of Medical Microbiology and Hygiene, Institute of Virology, Medical Faculty “C. G. Carus”, Technical University of Dresden.

3D microfluidic system for flow-based chemiluminescence analysis

The generation of chemiluminescence (CL) by aggregated gold nanoparticles is a cost-efficient alternative to enzymes. We use the effect of the prevention of aggregation by aptamers. Especially, *m*-carboxyl luminol has shown a significant signal enhancement compared to the hydrophobic luminol. A microfluidic flow-injection aptamer-based CL analysis system was developed which was able to quantify sulfadimethoxine with a limit of detection of 4 pg/mL.



Microfuidic fow-injection aptamer-based chemiluminescence platform.

State of the Art Aptamers are single-stranded DNA or RNA oligonucleotides that can specifically bind to various analytes similar to antibodies. Aptamers can be produced in large quantities through chemical synthesis. In combination with AuNPs, it provides the possibility for homogeneous CL assays which simplifies test protocols.

Analytical Approach A certain amount of salt can cause aggregation of AuNPs to enhance the CL signal. Aptamers interact with AuNPs leading to inhibition of the aggregation and resulting in a weak CL signal. Based on this mechanism, a homogeneous aptamer-based assay was developed in a microfluidic CL flow-injection platform with AuNPs as the catalyst for analytical applications. As efficient mixing of reagents in a microfluidic platform is crucial, a new laminated 3D microfluidic mixer was developed for our microanalytical system. The 3D micromixer was composed of two pressure-sensitive adhesive tapes and three PMMA layers.[1]

Results The hydrophilic *m*-carboxyl luminol[2] can achieve higher quantum yields compared to standard luminol and, in combination with gold nanoparticles, is very efficient in generating chemiluminescence. Analytes, aptamers, AuNPs, and *m*-carboxy luminol were mixed in the microfluidic channels for this homogeneous assay. Sulfodimethoxine was measured on the platform as an example via its aptamer and yielded a broad dynamic range over 5 orders of magnitude (0.01–1000 ng/ml) with a limit of detection of 4 pg/ml. This new detection concept can be suggested as a new flow-injection strategy for aptamer-based rapid and cost-efficient analysis in environmental monitoring and food safety

Yanwei Wang and Michael Seidel

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Prof. Antje Bäumner, Universität Regensburg

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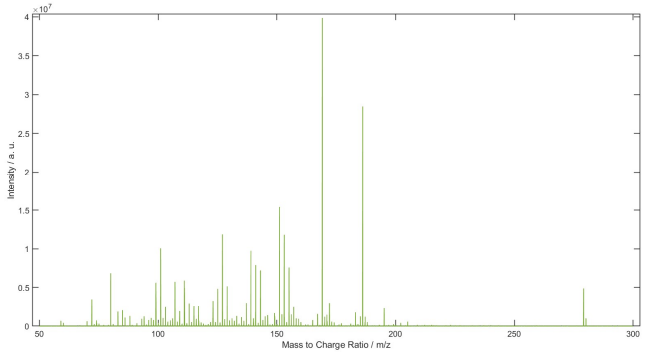
Chemical Characterization of Atmospheric Ultrafine Particles by Laser Desorption - Mass Spectrometry

Ultrafine particles (UFPs) have been proven to negatively affect the human health, mainly dependent on the chemical composition of the particles. This necessitates a reliable method for day-to-day qualitative analysis.

State of the Art Multiple techniques for the chemical analysis of atmospheric particles have been developed in the last decades.[1,2] For long-term monitoring, off-line sampling strategies offer a cost-efficient solution. The lack of simple and fast methods for the analysis of off-line UFP samples with mass spectrometry motivates the development of new desorption methods in the scope of this project.



Mass spectrum of a laser desorbed impactor collection with a mean aerodynamic diameter of 95 nm.

Analytical Approach Atmospheric particles were collected with an electrical low-pressure impactor (ELPI) on aluminum substrates. For preliminary experiments, the HELIOS IR-heating device was employed, which was previously developed in this group for the thermal desorption of the sample. To reduce measurement times and and improve reproducibility, a computer-controlled laser desorption setup was designed. Equipped with a 10.6 µm, 40 W laser and optics mounted to a XY-stage, it is possible to vaporize the volatile components of the sample. These compounds are then ionized by an SICRIT ion source from Plasmion GmbH, Augsburg, the start-up company founded by IWC-alumnus J.-C. Wolf, and subsequently analyzed with an Orbitrap Exactive mass spectrometer. In addition to that, samples were measured by SEM-EDX before and after laser desorption mass spectrometry in order to evaluate the change in elemental composition.

Results Our system for the laser desorption of ultrafine particles in combination with highly sensitive DBDI mass spectrometry allowed for both identification of the volatile fraction, as well as monitoring of substances of interest such as polyaromatic hydrocarbons. SEM-EDX confirmed a high efficiency of the laser desorption.

Felix Ludwig, Nico Chrisam, Kevin Maier

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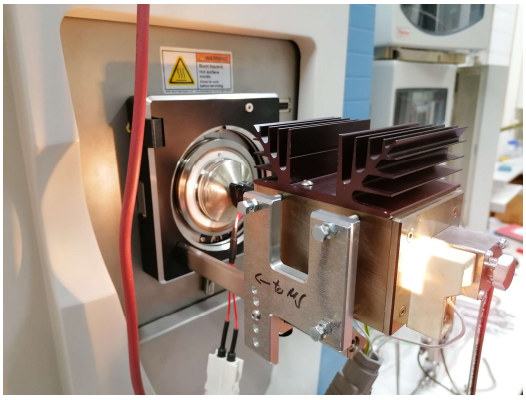
Cooperation
Bayerisches Landesamt für Umwelt (LfU)

Chemical Characterization of Atmospheric Ultrafine Particles by Thermal Desorption - Mass Spectrometry

Atmospheric particles are of great importance for the earth's water cycle and radiation balance. By acting as condensation nuclei for water vapor, they induce cloud formation and sustain life on earth. At the same time, they pose a health risk and could play an important role in climate change.[1] For all those processes, the chemical composition of the particles is essential.

State of the Art Instruments for both on-line and off-line analysis have been established for assessing the elemental and molecular composition of atmospheric particles. Mass spectrometric approaches cover a wide range of possible analytes with high sensitivities and provide insight into the variety of organic species.[2] Still, elaborate sample preparation with solvent-based off-line methods, or stationary equipment used in on-line techniques hamper their use in day-to-day monitoring of atmospheric particles for different locations.



HELIOS-SICRIT-HRMS system during a measurement of an ELPI-collected atmospheric particle sample.

Analytical Approach Atmospheric Particles were collected on aluminum substrates with an electrical low-pressure impactor (ELPI). The loaded aluminum substrates were introduced into a modified HELIOS-desorption cell previously developed within the group. By IR-heating, the volatile and semi-volatile species were desorbed from the substrate and introduced into an Orbitrap high-resolution mass spectrometer (HRMS). For ionization, the SICRIT ion source from Plasmion GmbH, Augsburg, the start-up company founded by IWC-alumnus J.-C. Wolf, was used. The measuring performance was evaluated with pure substance and propane soot test samples.

Results With our HELIOS-SICRIT-MS system, a first insight in the composition of ELPI collected atmospheric particles could be achieved. By data evaluation using van-Krevelen diagrams, a differentiation between natural and anthropogenic sources was indicated. However, long downtimes between the measurements for cooling of the desorption cell call for further development of the system.

Kevin Maier, Felix Ludwig

Funding

Bayerisches Landesamt für Umwelt (LfU)

Cooperation

Bayerisches Landesamt für Umwelt (LfU)

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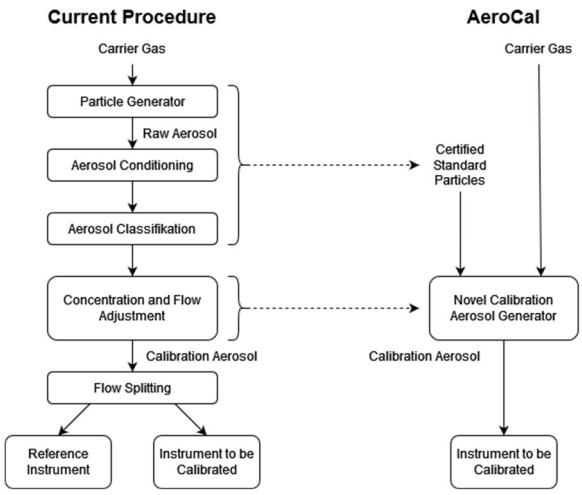
AeroCal – Calibration Aerosol Generator

For quality assurance, measuring devices should be calibrated regularly. Especially with aerosols, the calibration of measuring instruments requires extensive equipment to produce reliable calibration standards.

State of the Art The production of different calibration aerosols is described in VDI standard 3491.[1] An overview of the typical steps is shown in the left of the adjacent scheme. The type and size of the produced aerosol depends on the used particle generation method, which must be selected according to the individual requirements. Further conditioning, such as drying and electrical neutralization, can be needed to obtain a well-defined calibration aerosol. Also, gaseous, semi-volatile, or particulate interferents originating from the production should be removed. By classification of the particles, a narrower size distribution can then be generated. To ensure that the produced calibration aerosol meets the requirements, analysis with a reference instrument is also necessary.[2]

Analytical Approach The goal of this project is the development of an aerosol generator that can easily be used for the calibration of aerosol measuring instruments. In the aerosol generator, certified standard particles should be dispersed to directly deliver the desired aerosol concentration and size distribution, as shown in the right of the adjacent scheme. For that, a reliable method to deposit the particles in containers needs to be developed. Also, a method for redispersing the particles in a controlled manner without altering their shape is to be found. Then, a prototype of the calibration aerosol generator should be built and tested for its performance.



Scheme of the necessary steps in calibration aerosol production for aerosol instrument calibration. Left: Classical calibration. Right: Calibration with the novel calibration aerosol generator developed in this project.

Results First experiments on the particle production and conditioning have been conducted. Also, the produced particles were deposited on a surface and investigated with SEM.

Kevin Maier

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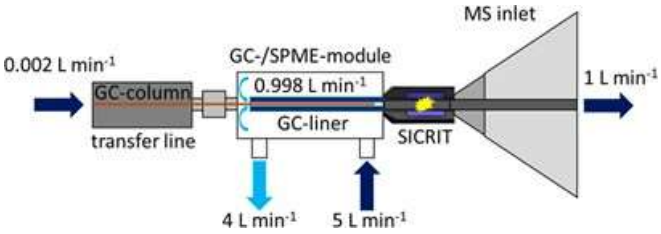
Characterization of SICRIT-Ionization

SICRIT is a versatile ionization technique for a wide variety of different compound classes ranging from non-polar components like alkanes and PAHs to highly polar amines, nitrosamines and nitro-compounds. At least three different ionization mechanisms are known and were characterized for different reactant gases.

State of the Art Currently, the SICRIT ionization source is applied for a wide variety of different compound classes, while the underlying ionization mechanism and influence of different reactant gases has been investigated only for limited compound classes such as PAHs[1] and alkanes.[2]



Schematic drawing of the GC-SICRIT-MS coupling. Compounds are separated via GC and enter the ionization source one at a time, while the atmosphere is controlled by an overflow of reactant gas.

Analytical Approach High resolution mass spectrometry allows to determine the elemental composition after ionization via SICRIT. Coupled to a GC, a mixture of different compound classes (e.g. alkanes, alkenes, PAHs, OMEs, esters, amines, phenols) could be examined in a single run under identical ionization conditions. Complete separation of the components allows clear assignment of the resulting ionized species to individual compounds. Eight different reactant gases/dopants (dry nitrogen, humidified nitrogen, room air, methanol, hexane, ammonia, HCl, fluorobenzene) were tested.

Results Ionization of about 120 different components in the presence of eight different reactant gases was investigated. The resulting data show an interesting behavior of certain compound classes, such as formation of ammonium-adducts for ethers or radical ionization of PAHs in the presence of fluorobenzene. Simultaneous monitoring of reactant ions like H_3O^+, NO^+, O_2^+ allows to determine possible ionization pathways.

In the future, we are going to expand the number of different compound classes, investigate behavior in negative ionization mode and compare sensitivity of different mass spectrometers. In addition, the data shall be fed into a database to enable everyone to choose the optimal ionization conditions for certain compound classes, or to identify unknown components.

Markus Weber

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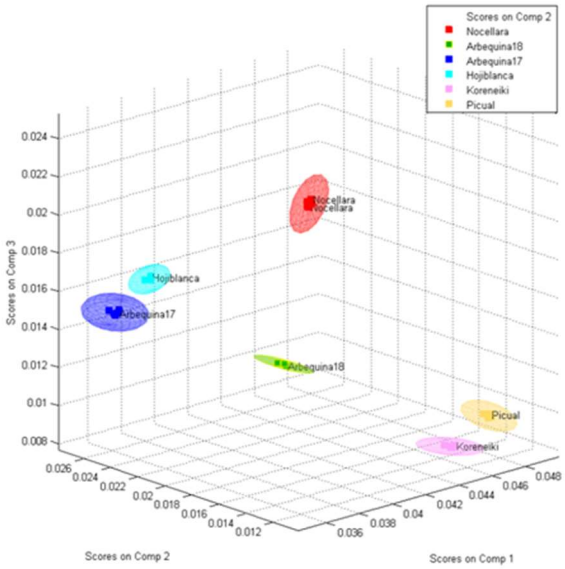
Plasmion GmbH,
IWC

Spectroscopic Characterization of Olive Oil

Spectroscopic techniques such as fluorescence, UV-VIS, Raman, and FTIR allow for rapid, relatively inexpensive, and easy analysis of olive oils regarding important quality criteria and abnormities. By employing chemometrics, classification regarding adulteration and oxidation can be achieved and may help in establishing less cumbersome alternatives to traditional means of fraud detection.

State of the Art According to a 2013 report by the European Parliament, extra virgin olive oil (EVOO) ranks in first place of food products at risk of being fraudulent.[1] For evidence, European legislation adopted almost exclusively chromatographic methods coupled with mass spectroscopy, which are both time-consuming and ill-suited for businesses without the means to access such expensive laboratory equipment for quality control.[2] Thus, to aid the goal of limiting fraudulent mislabeling that may result both in health risks as well as economic damages for consumers, additional data is warranted to bring forward promising alternatives alongside established techniques. Recently, a variety of successful attempts using a combination of spectroscopy and chemometrics have shown great promise.



3D scoreplot of PARAFAC analysis of Mediterranean olive oilvarietals (*Rapid Extra Virgin Olive Oil Classification and Blend Quantitation; Horiba Scientific: 2019).*

Analytical Approach Sets of measurement series are recorded to allow for a controlled variation of parameters of interest, and hence subsequently facilitate meaningful classifications in terms of adulteration and parameters related to refining, aging, or subpar storing conditions. Additionally, several monovarietal EVOOs will be evaluated regarding discriminability. Chemometric methods employed will likely include, but may not be limited to PARAFAC, PLS-DA, and PCA.

Results Preliminary data show that several oils commonly used in olive oil adulteration show characteristic deviations from spectra obtained from EVOOs. Parameters such as pigment content, oxidation state, and fatty-acid profile appear to be adequately captured by the respective spectroscopic methods employed. Further advances in chemometrics will be required to provide a basis that may allow for reliable interpretations in the future.

Jonas Flechtner

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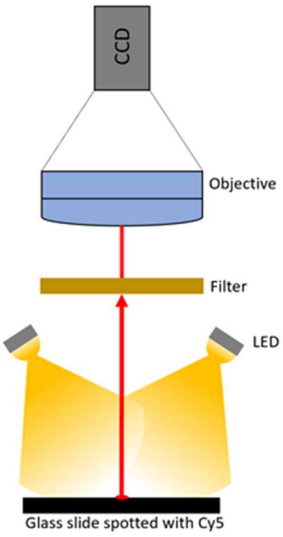
Funding
IWC

DetectRespi – Point-of-care diagnostics for respiratory infections

Development of a molecular biological Lab-on-a-Chip platform for the highly parallel detection of viral and bacterial pathogens of respiratory diseases. The molecular biological basis of this platform is a multiplex PCR coupled to a DNA microarray.

State of the Art Currently, there are a few Point of Care (PoC) diagnostic systems that work based on molecular biology. Disadvantages of these systems are often low multiplexing grades and high costs regarding the consumables and the operating devices. In addition, manual intervention and the need for different sample matrices make the use of these platforms inconvenient.



Schematic illustration of the optical read-out unit of the operating device developed within the project DetectRespi. The unit is based on a CCD-camera, an optical bandpass filter (670 nm) and LEDs (Exc.: 645 nm).

Analytical Approach The work on the biochemical assays of this project is executed by the institute of Division of Infectious Diseases and Tropical Medicine (LMU). The main tasks are the preparation of primers and probes for the panel and the development and preparation of the individual assay steps. For the implementation of a multiplex PCR, three steps are necessary: the decision on the aimed organisms of the panel, research about suitable targets in the genomes of the target organisms, and the design of primers. The cloning of PCR positive controls supports the work on testing primers and multiplexing them. The main task of the TUM is the design and realization of the optical read-out unit for the DNA microarray. The evaluation of the array will be done by fluorescence labeling of the PCR products using Cy5. Construction of the unit includes the choice of the best-suited camera module, the integration as well as the illumination tasks to allow for an optimal excitation and read-out. Thus, glass slides spotted with different concentrations of Cy5 and in different geometries are used for experimentation.

Results Five of the final 18 primer pairs of three organisms are designed and tested on functionality. Further primers are designed and have to be evaluated using organism-specific DNA. Multiplexing of primers and the evaluation of the primers in combination with patient samples are the next working steps. Regarding the optical readout of the DNA microarray, the experimental starting points are a CCD-camera, an optical filter (670 nm bandpass filter), and LEDs with an excitation wavelength of 645 nm. For optimal illumination of a sample, different components are constructed that help to generate a reproducible alignment and measurement. This setup is further optimized, refined, and adapted to the technical requirements.

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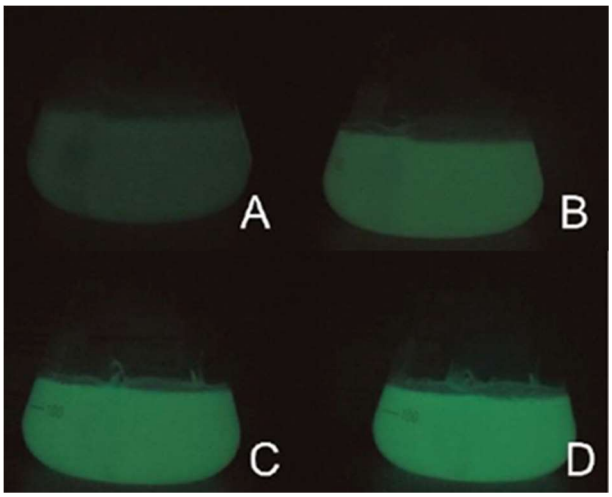
Eva Krois, Amelie Hohensee

Use of *Aliivibrio fischeri* as non-target toxicity test

The inhibitory effect of different environmental water samples on the luminescence of *Aliivibrio fischeri* as a test organism is used to develop a fast non-target toxicity test for the analysis of wastewater from fire extinguishing operations.

State of the Art *Aliivibrio fischeri* (*A. fischeri*) is a bioluminescent marine bacterium. It is used for toxicity tests of multiple environmental samples, like wastewater (according to DIN EN ISO 11348-1). For the fire brigade, it is of high importance to analyze the toxicity of fire extinguishing water to know if purification steps need to be taken. Here, the establishment of a non-target toxicity test using *A. fischeri* could generate a fast method to fulfill these requirements.

Analytical Approach Based on existing methods, experiments are set up to measure the inhibitory effect of different samples of fire distinguishing water on the luminescence of *A. fischeri*. Different growing conditions, such as the nutrition composition of the medium, were tested to establish a protocol to culture *A. fischeri*. Furthermore, reproducible fire extinguishing water samples were generated. Kinetic measurements are executed by measuring the inhibitory effect on the luminescence within 30 minutes of exposition.



Luminescent culture of *A. fischeri* at different optical densities: OD_{600} = 0.272 (A), OD_{600} = 0.416 (B), OD_{600} = 0.499 (C), OD_{600} = 0.529 (D).

Results To set up a method, the limits of the viability of *A. fischeri* during measurements are examined first. It was found that a concentration of 30 g/L sodium chloride is suitable to avoid a hypotonic shock of the bacteria and concurrently does not affect the luminescence of *A. fischeri*. Furthermore, the influence of water samples with different pH values on the viability of the bacteria was tested. The chosen pH range from 3.5 to 9.0, which coincides with the measured pH values of the fire extinguishing water samples, does not have a measurable effect on the luminescence of the bacteria. A concentration of 500 mg/mL zinc sulfate heptahydrate was examined as a suitable positive control for the test. The produced fire extinguishing water samples, originating for example from latex or motor oil, do not harm the viability of the bacteria. In contrast, the extinguishing foam which is used by the fire brigade has an inhibitory effect on the luminescence of the bacteria. In the future, it is planned to analyze more water samples as well as known toxic substances for further evaluation and improvement of the method.

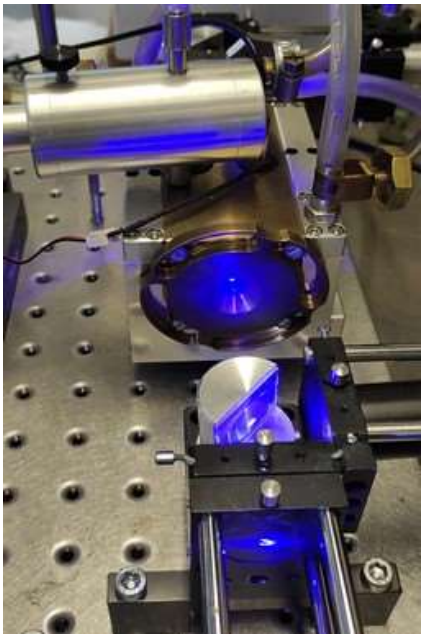
Amelie Hohensee, Eva Krois, Sarah Prakesch

Funding
IWC
Cooperation
Analytische Taskforce der Feuerwehr München (ATF)

Fundamentals of Aerosol Photoacoustic Spectroscopy

Evaporation of volatile substances from aerosol particles can influence their signal properties in photoacoustic analysis. Previous theoretical studies considered the evaporation process of water under strict approximations. This experimental work used stearic alcohol as a more realistic compound of higher molecular mass. For soot particles, the photoacoustic signal showed indeed a shift in the resonance frequency.

State of the Art Photoacoustic spectroscopy (PAS) has been developed as a way of measuring the light absorption of aerosol particles. A modulated light source hits the particles and sound waves are produced as the heat is transferred to the surrounding gas. Consequently, the acoustic signal may be modified when particles are surrounded by different substances. For instance, calculations under specific boundary conditions have described how a PA signal can be influenced by water evaporation.[1] Moreover, literature contributions report how the gas sample composition (like different relative humidity levels) can influence the photoacoustic signal characteristics.[2]



Experimental setup for PAS: resonator cell at controlled temperature and laser diode emitting in the blue range.

Analytical Approach The main goal of the experiment was to check whether and how the interaction between laser and coated particles could modify the PA signal. The evaporation of the coating determines an overall variation of the gas inside the PA cell. To study the PA signal when particles are surrounded by volatile compounds, soot particles coated with stearic alcohol were used as samples and Argon as carrier gas. The PA setup used a solid-state laser with λ = 447 nm and an emitting power of 800 mW.

Results Coating evaporation was expected to modify the resonant frequency of the PA signal. Therefore, a frequency scan from 3.3 to 3.9 kHz was performed. The resonance peak of the PA signal in presence of evaporated compounds was shifted by about 4 Hz to a lower frequency relative to the peak detected from uncoated particles. This observation is in agreement with the change in the speed of sound in the case of propagation through media with a heavier molecular mass. On the other hand, the amplitude of the PA signals grew linearly with the particle concentration with and without coating.

Emilio Ambra

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Funding

Deutsche Forschungsgemeinschaft (DFG)

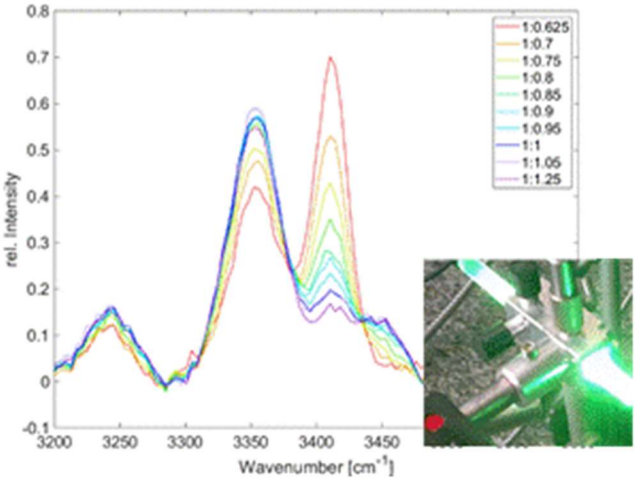
Cooperation

ETH Zürich

Process analytics with Raman and Fluorescence spectroscopy in flow reactor systems

For continuous reaction monitoring, in-line Raman and fluorescence spectroscopy are employed simultaneously with a modified Raman probe adapter. The approach was successfully evaluated with various vegetable oil mixtures and for monitoring of reaction products in nitration of aromatic substrates in microflow reactors.

State of the Art For reaction and process monitoring, in-line Raman spectroscopy is a fast alternative to offline GC-MS, enabling real-time and in-situ analysis. Based on the spectral fingerprint and sophisticated data analysis, different parameters, such as reactant consumption, product formation, and variations in reaction conditions, can be analyzed simultaneously. Compared to offline analysis, online spectroscopy measurements are faster and require no sample preparation.



Raman spectra of guanidinium carbonate (3414 cm^{-1}) and nitroguanidine (3360 cm^{-1}) during nitration with different molar ratios ($Z(G^+):Z(HNO_3)$). Inset: Raman probe adapter for in-line Raman and Fluorescence spectroscopy

Analytical Approach A previously developed adapter that is constructed to fix a Raman probe head to the tube of the microflow reactor was modified to allow simultaneous fluorescence measurements perpendicular to the Raman laser beam. In this setup the focus of the Raman laser lies exactly in the process flow. The spectra are processed by MATLAB (R2020b) to monitor the temporal evolution of educt and product concentrations. A CW laser (532 nm) is used as excitation source. The investigated reaction was the nitration of guanidinium carbonate to nitroguanidine in a mixture of concentrated sulfuric and nitric acid. In a second application, the possible application of simultaneous Raman and fluorescence measurement was evaluated with anaylsis of different olive oil and sunflower oil blends in the flow.

Results The Raman probe adapter was successfully optimized to measure Raman and fluorescence spectroscopy simultaneously in a PFA tube of the reactor system. By combining both spectroscopic techniques, the setup allowed different olive/sunflower mixtures to be analyzed and differentiated by specific signals. As monitoring of the reactants and nitro compounds was feasible with this in-line Raman spectroscopy in a continuous flow, the influences of various reaction parameters, such as reaction temperature, total flow rate, and stoichiometry of the reactants, on product formation were studied. The yield was determined using a calibration curve. The intensities of prominent bands of the substances were selected for the calibration.

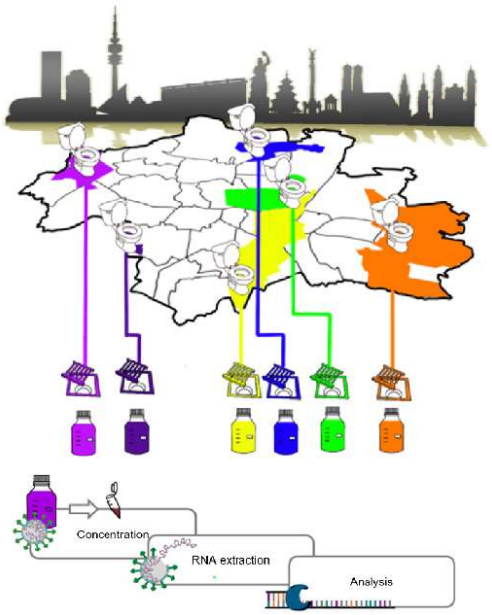
Lucas Hirschberger

Funding
IWC
Cooperation
Department of Chemistry, Energetic Materials Research, Ludwig-Maximilian University of Munich

Spatially resolved qualified sewage spot sampling to track SARS-CoV-2 dynamics in Munich[1]

The routine analysis of qualified spot sampled sewage once a week from six locations enables the tracking of SARS-CoV-2 dynamics in Munich over one year.

State of the Art Wastewater-based epidemiology (WBE) is a tool to monitor the SARS-CoV-2 burden in populations without the need for individual mass testing, especially in metropolitan areas.



Workflow to test if a weekly qualified spot sampling of the sewage system of six neighborhoods in Munich is sufficient to detect and track the local distribution of SARS-CoV-2

Analytical Approach We chose to perform qualified spot sampling of sewage once weekly in six different positions in the Munich sewage system, covering close to one-third of the population of the city (504,807/1,560,042 inhabitants; 32.4%). To keep the protocol convenient and cost-efficient, filtration with stainless steel strainer and subsequent ultracentrifugation was used to concentrate SARS-CoV-2 for RNA isolation. Viral load measurements were performed with RT-qPCR and digital droplet RT-PCR (ddRT-PCR) against two independent target genes. A subset of RNA eluates was also sequenced after PCR amplification to analyze viral genomic information.

Results Sewage SARS-CoV-2 RNA-load aligns well with the notification numbers in all six regions. However, the variation of notification numbers and the SARS-CoV-2 RNA-load in the sewage over time is considerable. It can be appreciated that the sewage RNA load precedes the notification numbers by roughly three weeks. Additionally, we performed sequencing to obtain information about the prevalence of variants of concern within the population, for example, the prevalence of B1.1.7. For B.1.1.7, we detected sustained levels of key mutations in wastewater beginning around week 3 of 2021 and reached an average representation of about 60% around week 7. Similar proportions were only reached in sequenced patients' swabs around week 10. The sewage sequencing was able to predict a subsequent increase of B.1.1.7 in the population, similarly to what was observed with case numbers in our study and others.

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Funding

Bavarian State Ministry of Science and the Arts

University Hospital of the LMU Munich

Cooperation

Max von Pettenkofer Institute & Gene Center, Virology, LMU Munich

Munich Metropolitan Sewer Authority, Munich

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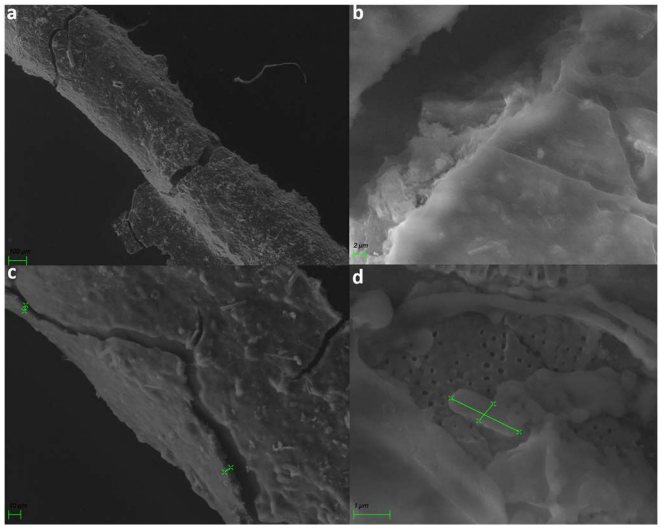
Characterization of biofilms used in microbial fuel cells with Raman- and SEM-based techniques / RAMBo

Exploring the potential of Raman microspectroscopy and scanning electron microscopy for the analysis of chemical composition and structure of biofilms from microbial fuel cells

State of the Art Wastewater treatment in the brewery sector is a highly energy consuming process, which also leads to the production of greenhouse gases as a second major side-effect. Intermediates of the anaerobic wastewater purification process can be used as a substrate feed for microbial fuel cells (MFC), making wastewater treatments less energy-consuming by producing bioelectricity as an innovative approach.[1]



Anode covered with thick biofilm (a + c), visualization of the 3D biofilm structure with different layers of the biofilm (b + c), visualization of rod-shaped bacteria (d; < 2 µm).

Analytical Approach The project focuses on the analysis of biofilms using imaging methods such as scanning electron microscopy (SEM) and Raman microspectroscopy (RM) to aid in elucidating the mechanisms of electricity production in MFCs. RM enables the spatial *in situ* study of chemical biofilm components at different stages of biofilm growth. SEM complements the information obtained by RM with high-resolution imaging of the three-dimensional structure of biofilms.

Results To monitor the stages of the biofilm development, several graphite fibers (parts of MFC anode) were removed from the MFC. After a drying process these fibers were analyzed with SEM. The examination at and below the micrometer scale pictured the formation of a three-dimensional biofilm structure, including cells with different shapes and sizes (round and rod-shaped) and inorganic particles. It can be deduced that the biofilm was built in layers over time and is harboring a variety of organic and inorganic materials. Raman analysis revealed biomass spectra with signals that can be mainly assigned to a) bacterial cells, b) polyhydroxybutyrate, produced as a polymeric substance for energy preservation as a stress response on nutrient depletion of bacteria, and c) carotenoids produced by bacterial cells. Chromophores, such as carotenoids, can be used as possible electron shuttles for electricity generation, as they can be reduced and oxidized during the process of electron transfer to a conductive surface.

Irina Beer

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Funding

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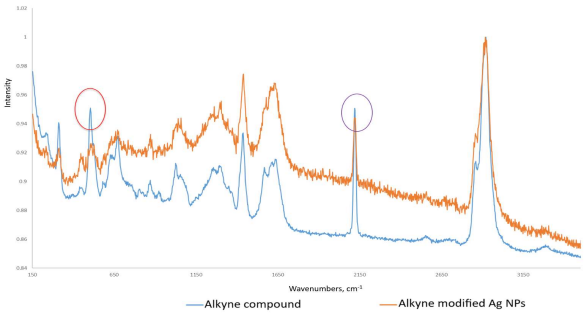
Cooperation

Prof. Dr. Thomas Hofmann, Dr. Karl Glas (Water System Engineering, Chair of Food Chemistry and Molecular Sensory Science, TUM School of Life Sciences Weihenstephan)

Synthesis of alkyne-modified silver nanoparticles for cell capturing and characterization by Raman analysis

Alkyne modified silver nanoparticles (Ag NPs) were synthesized to develop targeted anchors for active cells through Click reaction-based chemistry for subsequent Surface-enhanced Raman Spectroscopy (SERS) analysis.

State of the Art Ag NPs are used in SERS to enhance the Raman signal and to gain more specific information about target analytes in comparison to regular Raman microspectroscopy (RM). In particular, while Ag NPs can be applied for SERS analysis of living cells such as bacteria[1], so far they work in a non-targeted fashion. Alkyne-modified Ag NPs can interact in azide-alkyne cycloaddition "click" reactions offering a promising strategy for targeted detection of active cells.[2] The aim of the study was to optimize conditions for the synthesis of alkyne-modified Ag NPs and characterize products via RM.



Raman spectra of the alkyne modifying compound (blue) and alkyne modified AgNPs (orange).

Analytical Approach The alkyne-containing precursor compound for surface functionalization *5-(1,2-dithiolan-3-yl)-N-(prop-2-ynyl)* was synthesized according to Shi et al.[3] and characterized via nuclear magnetic resonance, Orbitrap mass spectrometry and RM. Then, Ag NPs were brought to reaction with the activated precursor compound and thoroughly washed with *tert*-butanol and water. Subsequently, particles were characterized by RM as rapid, minimally invasive and sensitive approach to confirm the success of covalent binding of *5-(1,2-dithiolan-3-yl)-N-(prop-2-ynyl)*.

Results Binding of the alkyne-containing precursor compound to Ag NPs is accompanied with a cleavage of S–S in the dithiolane cycle of the alkyne compound and formation of Ag–S bonds. It is followed by decrease of the Raman peak intensity at 502 cm^{-1} corresponding to S–S stretching in the target compound. Ag–S bonds are reflected in the Raman band at 240 cm^{-1}, whereas alkyne groups are observed as the Raman band at 2121 cm^{-1} in both alkyne modifying and target compounds. To find the optimal conditions for synthesis of the modified NPs, different durations of coupling and washing steps were tested.

Oleksii Morgaienko

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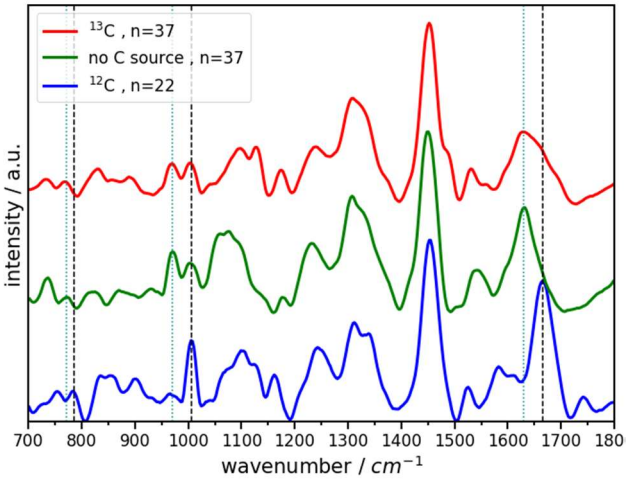
Funding
IWC-TUM

Potential of stable isotope Raman microspectroscopy for the analysis of biodegradation of microplastics

The applicability of stable isotope Raman microspectroscopy (SIRM) to track stable isotope labels from microplastic (MP) particles into microbial biomass is presented. Incorporation of heavier isotopes can be detected by a redshifted Raman signal.

State of the Art Indirect methods for the analysis of biodegradation of plastics focus either on analyzing properties of the remaining polymer or on the monitoring of metabolites. Recently, ^{13}C-labels were directly tracked from the polymer into microbial biomass with NanoSIMS (Secondary Ion Mass Spectrometry).[1] While providing very high resolution, NanoSIMS is expensive and requires elaborate sample preparation motivating the need for SIRM as simpler approach with additional structural data on a single cell level.



The fingerprint region of the mean spectrum of initially ^{13}C-labeled *S. koreensis* cells (green) is compared to the reference mean spectra of ^{13}C- (red) and ^{12}C- (blue) cells, after incubating the sample in carbon-free medium for 12 weeks. Three distinct bands and their redshifted analogs are marked with dashed lines, and all match the ^{13}C-signals for the sample.

Analytical Approach Our goal is to use ^{13}C-labeled polymers to monitor the carbon uptake of bacteria. Since ^{13}C-label is expensive, in a first approach we spearhead the method with D-labeled polymers. Inverse labelling is another cheap alternative. Here, cells are initially labeled with ^{13}C-glucose before they are transferred into carbon-free medium with microplastic (MP) particles, so that dilution of the ^{13}C-label by ^{12}C from the MP particles indicates degradation.
First experiments were conducted with bacteria of *Sphingomonas koreensis*, which had been isolated from polylactide acid (PLA) particles in an environmental sample. The bacteria contain carotenoids, which allow resonance Raman analysis with a short integration time of 1 s and a laser power of 1 mW at the sample due to their chromophoric diene system.

Results ^{13}C- and D-labeling of *S. koreensis* was successfully performed with ^{13}C-glucose and D_2O as substrates and the corresponding redshifted signals were shown to differ between non-labeled and labelled cells with resonance and regular Raman microspectroscopy. Furthermore, experiments with initially labeled ^{13}C-cells and carbon-free medium showed no dilution of the label during an incubation time of 12 weeks (see Figure). This provides promising results for a reverse labeling approach.

Kara Müller

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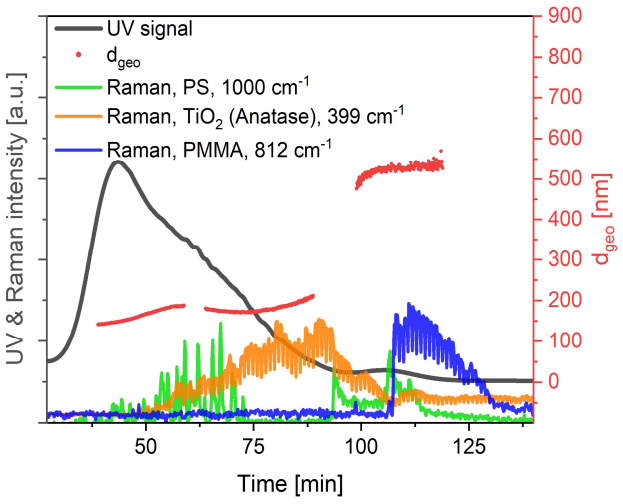
Cooperation
Dr. Michael Sander, ETH Zürich
Dr. Tillmann Lüders, Universität Bayreuth

Online-coupling of Raman microspectroscopy and field-flow fractionation: Towards the analysis of real samples

An optimized, online-coupled field-flow fractionation (FFF) Raman microspectroscopy (RM) setup was used to investigate particles that mimic typical environmental analytes. To this end, suspensions of particles were prepared that show high polydispersity, a non-spherical shape, and which represent different material properties.



Online FFF-RM analysis of a mixture of polystyrene (PS, 140 nm, spherical), titanium dioxide (polydisperse, irregular shape) and poly(methyl methacrylate) (PMMA, 500 nm, spherical) particles.

State of the Art It has been demonstrated that online-coupled FFF-RM can provide size-resolved chemical analysis of nanoplastics and other particles down to 200 nm.[1] However, the properties of environmental samples are expected to differ from the previously investigated particles, especially in shape, polydispersity, and surface chemistry. Thus, the need arises for the analysis of more realistic reference materials.

Analytical Approach The optimized online-FFF-RM setup allows for particle detection in a size range that is not fully accessible to common optical microscopy methods.[1] Specifically, the FFF system is used to separate particles in the size range of 100 nm to 5 µm where a multiangle light scattering (MALS) detector can provide corresponding size information. A custom-designed flow cell enables the chemical characterization of particles via Raman microspectroscopy using optical forces.

Results The analysis of a mixture of inorganic particles (TiO_2) and nanoplastics (polystyrene, PS and poly(methyl methacrylate), PMMA) was used to demonstrate the applicability of this method for the detection of nanoplastics in an inorganic matrix. While all spherical particles could be optically trapped in the flow cell, our experiments showed that rod-shaped particles cannot be trapped with the current setup due to their shape. Furthermore, the low density of polyethylene (PE) particles required a higher laser power for trapping due to the greater influence of hydrodynamic forces. These results indicate that further optimization of the setup is necessary, including sensitivity improvements, for the analysis of environmental samples.

Maximilian Huber

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Dr. Fanny Caputo, SINTEF Industry;
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References

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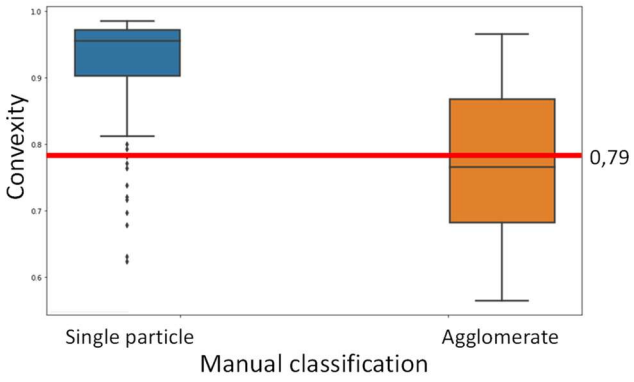
Adaptive watershed transformation as method for deagglomeration of objects during image analysis

While agglomeration of particles may create bias in numbers and size analysis, global deagglomeration may create bias by overcompensation. Here we suggest to select particles for correction based on conditions for brightness distribution and shape. These criteria can be derived from segmentation based on human expertise and used for automated adaptive deagglomeration of objects.

State of the Art Small particles, when present in agglomerates, may inadequately be detected as lager analytes. Deagglomeration algorithms like watershed transformation have therefore been brought forward for correcting obtained particle numbers. Although there are always singular cases for useful separations, recent work suggests that application of the algorithm to a whole sample leads to overestimation of particle numbers and fragmentation of fibres.[1,2] As an alternative, the method might also be guided or inspected manually.[2] However, missing reproducibility is considered as a disadvantage here.



Representation of separate convexity distributions for single particles and agglomerates after manual classification. The corresponding separating value is calculating by applying Otsu's algorithm.

Analytical Approach The particles to be analyzed are deposited on Au-coated track-edged membranes (polycarbonate (PC), 0.8 µm pore size), that are microscopically imaged. Using results of morphological measurements after object detection, *Otsu's* algorithm is applied to the convexity of single particles and agglomerates in consequence of manual classification. Afterwards, the threshold obtained from *Otsu´s* algorithm is used for selecting those objects on which watershed transformation is to be applied.

Results Objects with convexity below the threshold are subjected to deagglomeration. Before, an automated object classification for fibres is done so that they can be excluded from this procedure to avoid the problem of dissection. Preliminary results of an analysed image show a better approximation to manually counted particles (360 – 440) when comparing adaptive deagglomeration results (340) against the results without deagglomeration (230).

Oliver Jacob and Alejandro Ramírez Piñero

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Funding

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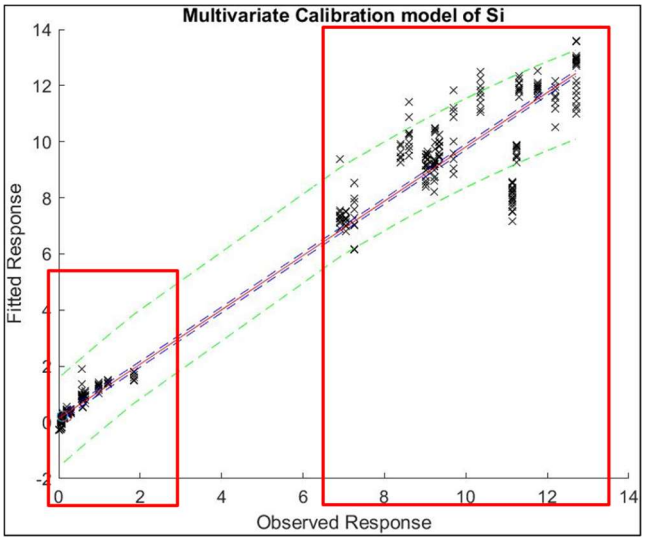
Cooperation

Aaron Beck, Eric Achterberg (GEOMAR, Kiel, Germany)

Development of LIBS calibration models for different elements in Al-alloys

Quantification of metal alloy composition can be hampered due to matrix effects and inhomogeneities – especially when analyzing particles with small volumes. Using multivariate (PLS) regression models, quantification of elements in Al alloy bulk and particle material is enabled.



Recovery function of the PLS calibration of Si. This model covering a wide concentration rage shows differences in high and low concentrations (red boxes), which can be assigned to matrix effects. To enable accurate analysis, the calibration therefore was split in sub-calibrations.

State of the Art All alloys show inhomogeneities dependent on several factors like elemental composition, production, heat treatments etc. These inhomogeneities hamper quantification, since varying matrices and elemental concentrations in the sample increase uncertainties in calibration models. Especially for the quantification of particle composition, where the small volume hampers multiple measurements, quantification can be a challenge – even for the small necessary volume for LIBS analysis. Therefore, both measurement and evaluation parameters must be optimized for the samples matrices, to ensure accurate and correct results.

Analytical Approach After optimizing LIBS measurement parameters on aluminum matrices, 60 certified reference materials were analyzed as training data. Univariate and multivariate (partial least square (PLS) regression) quantification models, with different normalization methods were developed and compared regarding their accuracy in validation measurements.

Results When comparing validation results of univariate and multivariate regression models, the latter was identified as the more accurate method. By normalizing to a weak signal, an improvement in the form of smaller deviations was obtained compared to normalizing to an intense signal. Due to a wide concentration range covered by some calibrations or strong matrix effects, quantification models were divided in sub-calibrations covering a smaller concentration range with a more linear behavior. Validation using certified reference material showed deviations within acceptable error, which confirms the functionality of the models. Additionally, used industrial components were characterized and differentiated. Further, particles of different sizes (from 1000 µm down to 45 µm) were successfully analyzed with the proposed models.

Funding
BMW Group

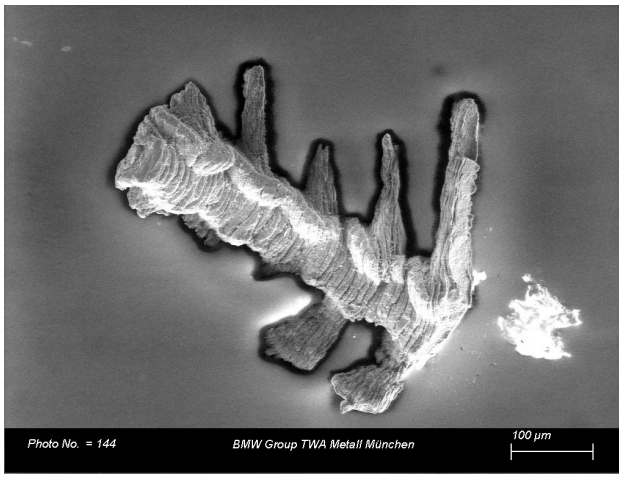
Cooperation
Laser Technik Berlin (LTB)

Maria Lanzinger

Generation of metal alloy reference particles and analysis regarding their size, morphology and elemental composition

Reference particles are invaluable when calibrating measurement equipment and validating analytic methods. To this end the production of size-sorted reference particles from alloys was attempted. Furthermore, as all alloys show inhomogeneities, the elemental composition of the particles was analysed and compared to the bulk material.

State of the Art Reference particles are needed for almost all experiments such as validating or calibrating analysis methods. However, currently reference particles are only available for a small number of materials and sizes. Furthermore, no reference particles are available for alloys as their elemental composition can vary greatly. The inhomogeneity of metal alloys due to effects such as heat treatment or segregation during the cooling process is a well-known problem in metal analysis. These problems can become more serious for particles as the particles have a small volume and certain elements tend to break out of alloys due to their brittleness when confronted with mechanical stress or pressure.



SEM image of a steel particle produced by the hand-held mortar as an example of the highly irregular shapes produced by this method.

Analytical Approach To solve this problem, reference particles were generated from real components used in the automobile industry by grinding shavings applying both a hand mortar and a vibratory disc mill. These particles were then sieved into size categories and analysed regarding their shape. To test if the production method and size of the particles have an influence on their elemental composition, particles were analysed via inductively coupled plasma optical emission spectrometry (ICP-OES), spark spectroscopy and laser induced breakdown spectroscopy (LIBS) and compared to the bulk material.

Results Using the proposed method, size-classified particles of three different materials were generated, validated by light microscopy and scanning electron microscopy (SEM) and then applied for the validation of different particle detection systems. The SEM analysis of the particle morphology yielded significantly more irregular shaping of hand-ground particles compared to the machine-ground particles. Depending on the size and production method, the concentration of certain elements was shown to vary up to 2 $\%_{wt}$ compared to the bulk material for Al-Si and steel. However, the elemental composition of brass particles matched the bulk material with differences of less than 0.1 $\%_{wt}$ for the alloyed elements.

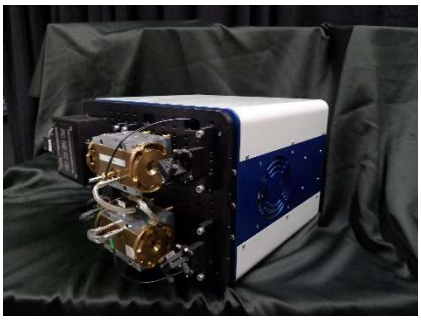
Alexander Thomas

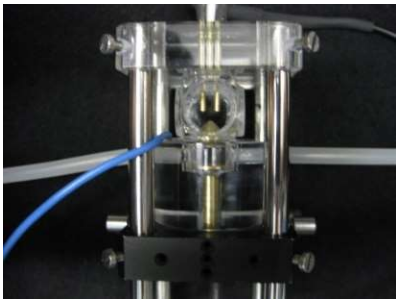
Funding
BMW Group

Cooperation
Lasertechnik Berlin GmbH

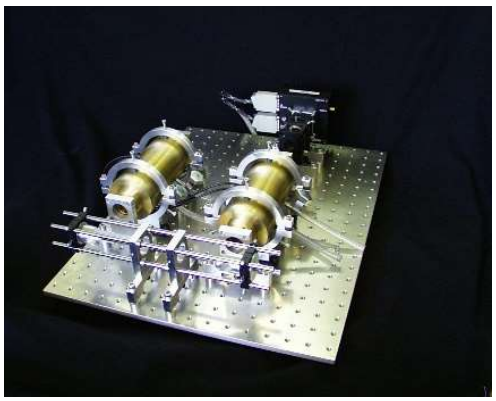
Good-Bye to our Mechanical Workshop

When Prof. Niessner accepted the professorship at TUM, he foresightedly established a fully equipped mechanical workshop in a separate building next to the institute's main building in Großhadern. But even he did most likely not anticipate how extremely valuable this installation, and even more so the specialists working there, would become for our research when Mr. Dollinger started to work there as first head and *Meister*.

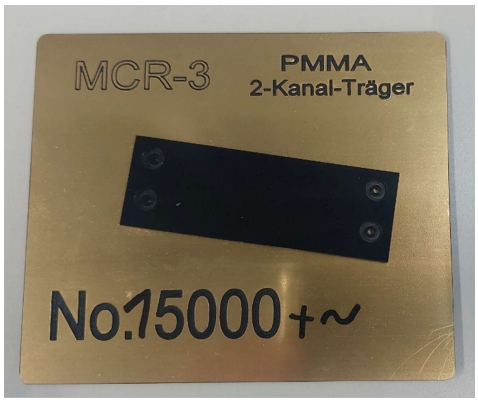


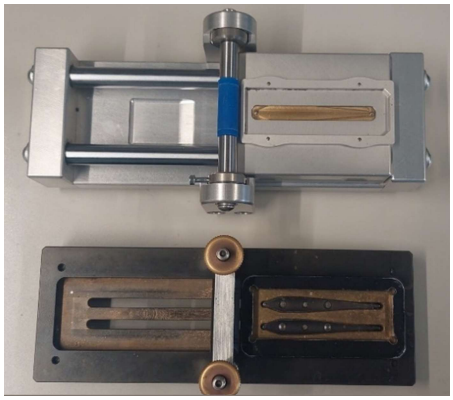


Over the years, the workshop's constructions became more and more complex, starting from purely mechanical parts to the development of complete instruments. Prototypes, suitable for routine use in industry, were developed and built. First prototype for "Munich Plastic Sedement Separator (MPSS)" is already included as an exhibit in the collection of Deutsche Museum. Later on, the workshop even included software programming and electronic layout and soldering into their full-service package. Eventually, they executed complete research projects, besides quickly stepping in as janitors. We were envied by colleagues from all over the world for this workshop (and that's no exaggeration, we heard that a lot from many visitors).



When, at the end of ’21, the last of us had to leave Großhadern on short notice with only 3 weeks to end all activities, we completely lost these unique possibilities, thus efficiently bringing to a stop a whole branch of our research work. While much can be said about the sense and nonsense of this high-up decision, we will leave it at saying a huge





Thanks to Roland Hoppe and Sebastian Wiesemann for Everything!

Christoph Haisch, Michael Seidel, Natalia Ivleva and Martin Elsner

Birgit Apel†

In November 2021 our institute member and technician, Miss Birgit Apel passed away. Miss Apel has served our institute for almost 40 years. She has been the soul of our water laboratory and has laid the hydrochemical foundation for generations of bachelor, master, and doctoral students. She was responsible for the analysis of hydrothermal bath, spring, and mineral waters. In the hydrochemistry block course she was a dedicated teaching assistant who showed generations of hydrogeology students how to work in analytical chemistry and water chemistry. She has worked with three institute directors. We thank her for dedicating her working life to the IWC and will keep her in fond memory.

Im November 2021 schied unser Institutsmitglied und unsere langjährige Technikerin Frau Apel von uns. Frau Apel hat unserem Institut seit fast 40 Jahren gedient. Sie war die Seele unseres Wasserlabors und hat die hydrochemische Basis für Generationen von Bachelorstudenten, Masterstudentinnen und Doktorierende gelegt. Sie war verantwortlich für die Analyse der hydrothermalen Bäder-, Quellen- und Mineralwässer. Im Hydrochemiepraktikum war sie eine Autorität für Generationen von Hydrogeologiestudierende, denen sie das praktische Arbeiten in Analytischer Chemie und Wasserchemie nahebrachte. Sie hat mit drei Institutsdirektoren zusammengearbeitet und ihr ganzes Arbeitsleben dem IWC gewidmet. Wir werden sie in ehrenvoller Erinnerung behalten.

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Conference Presentations

Oral Presentations

Auernhammer, A., Development of a multiplex algae toxin immunoassay for the monitoring of algal blooms in surface water, *Medical Biodefense Conference*, 29.09.-01.10.2021, München, Germany. Ivleva, N. P., Analysis of nanoplastics by Raman microspectroscopy-based methods. *SETAC 2021 Virtual Seminars*, 16.3-6.4.2021 (invited).

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Klüpfel, J., Rapid detection of (neutralizing) SARS-CoV-2 antibodies by chemiluminescence microarray immunoassay. *Medical Biodefense Conference*, 29.09.-01.10.2021, München, Germany.

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Poster Presentations

Auernhammer, Andreas.; Seidel, M., Kombinierung eines Wasser-Sensorsystems mit einem vollautomatischen indiretk kompetitiven Durchfluss-Microarray-Immunoassay als Frühwarn-System für vermehrtes Algenwachstum und Freisetzung von Algentoxinen in Oberflächengewässern. *Dresdner Sensor Symposium*, 06.-08.12.2021, online.

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Morgaienko, O.; Klein, P.; Elsner, M.; Ivleva, N.P., Raman analysis of the modified silver nanoparticles during their synthesis. *17th Confocal Raman Imaging Symposium*, 27.09-1.10.2021, (online).

Neumair, J.; Elsner, M.; Seidel, M., Flow-based chemiluminescence microfluidic chip to screen for affinity ligands for capturing bacteria. *European Biosensor Symposium*, 09.-12.03.2021, online.

Neumair, J.; Zheng, V.; Heller, S.; Würstle, S.; Obermeier, A.; Schneider, J.; Burgkart, R.; Elsner, M.; Seidel, M., Towards faster detection of pathogens in human body fluids: testing platform for affinity ligands for monolithic affinity filtration. *Medical Biodefense Conference*, 29.09.-01.10.2021, online.

Neumair, J.; Elsner, M.; Seidel, M., Testsystem zum schnellen Screenen von Affinitätsliganden zur Aufkonzentrierung von Bakterien. *Wasser 2021*, 10.-12.05.2021, online.

Schwaiger, G.; Seidel, M., Quantification of *Legionella spp.* by viability heterogeneous asymmetric recombinase polymerase amplification (v-haRPA) on a flow-based chemiluminescence microarray. *European Biosensor Symposium*, 09.-12.03.2021, online.

Schwaiger, G.; Seidel, M. Quantifizierung und Monitoring von *Legionella spp.* in biologischen Abluftreinigungsanlagen mittels Chemilumineszenz-basierter Detektion auf einem Mikroarray. *SETAC GLB Jahrestagung Umwelt*, 07.-08.09.2021, online.

Schwaiger, G.; Clauss, M.; Seidel, M., Isothermale Detektion von Legionellen mittels Lebensfähigkeits-haRPA in biologischen Abluftreinigungsanlagen. *Wasser 2021*, 10.-12.05.2021, online.

Schwaiger, G.; Seidel, M. Quantifizierung von *Legionella spp.* mittels isothermaler Amplifikation auf einem Chemilumineszenz-basierten Mikroarray. *Dresdner Sensor Symposium*, 06.-08.12.2021, online.

Streich, P.; Seidel, M.; Characterization and validation of screening methods for culture-independent detection of *Legionella* in artificial water systems. *European Biosensor Symposium*, 09.-12.03.2021, online.

Streich, P.; Biedermann, B.; Herr, C.; Lück, C.; Priller, F.; Redwitz, J.; Spindler, B.; Walser-Reichenbach, S.; Seidel, M.; Analytische Charakterisierung und Validierung von Schnellmessmethoden zur Detektion von *Legionellen* in wasserführenden technischen Anlagen. *Wasser 2021*, 10.-12.05.2021, online.

Streich, P.; Redwitz, J.; Harbich, E.; Biedermann, B.; Walser-Reichenbach, S.; Herr, C.; Lück, C.; Seidel, M.; Gestaltung eines Verbundprojektes für die Bereitstellung kulturunabhängigen Screeningmethoden zur Bestimmung von *Legionellen* Konzentrationen in technischen wasserführenden Anlagen. *SETAC GLB Jahrestagung Umwelt*, 07.-08.092021, online.

Streich, P.; Biedermann, B.; Redwitz, J.; Lück, C.; Seidel, M.; Characterization of culture-independent screening methods of the detection of *L. pneumophila* in artificial water systems. *Medical Biodefense Conference*, 29.09.-01.10.2021, online.

Invited Lectures

Elsner, M., Trace Analysis of Isotopes at Natural Abundance – Challenges and Opportunities. Inorganic Chemistry Seminar Series, Technical University of Munich, 8.9.2021

Ivleva, N. P., Raman Microspectroscopy for Analysis of Microplastics and Nanoplastics. Vrije Universiteit Amsterdam, 2.11.2021.

Haisch, C., HELIOS/SICRIT/MS: a new tool for aerosol analysis, AIMS live event, 8th of July, Beijing, China

Haisch, C., Thaler, K.M., Pang, G., HELIOS/SICRIT/MS: Exhaust analysis and more, Plasmion User Forum, online, 23.11.2021

Haisch, C., F. Ludwig, K. Maier, Chemische Charakterisierung von UFP aus Verbrennungsprozessen, Online-Fachtagung „Ultrafeine Partikel“, Bayerisches Landesamt für Umwelt 25.11.2021

Seidel, M., Kulturunabhängige Nachweisverfahren als Strategie für eine verbesserte Risikoanalyse von Legionellen in Verdunstungsrückkühlanlagen. Wasserchemie in Industriekraftwerken - TÜV Süd, 4.-5.10.2021, München.

Seidel M., Kulturunabhängige Nachweisverfahren als Strategie für eine verbesserte Gefährdungsanalyse von Legionellen in Verdunstungsrückkühlanlagen. VDI Wissensforum, 2.3.-3.3.2021, online.

Scientific Committees & Memberships

Elsner, M., Young Academy of Europe, YAE (Member)

Elsner, M., Wasserchemische Gesellschaft, Fachgruppe der GDCh (Vice President)

Elsner, M., Environmental Science & Technology (Member of the Editorial Advisory Board)

Elsner, M., ACS ES&T Water (Member of the Editorial Advisory Board)

Elsner, M., Journal of Isotopes in Environmental and Health Studies (Member of the Editorial Advisory Board)

Elsner, M., Evaluation Panel Member of the Swiss National Science Foundation

Elsner, M., Bayer. Fachausschuss für Kurorte, Erholungsorte & Heilbrunnen Member

Elsner, M., Dean of Studies, Faculty of Chemistry, Technical University of Munich

Elsner, M., TUM Water Cluster, Speaker, Technical University of Munich

Ivleva, N. P, ISO/TC 147/SC 2/JWG 1 "Joint ISO/TC 147/SC 2 - ISO/TC 61/SC 14 WG: Plastics (including microplastics) in waters and related matrices" (DIN Expert)

Ivleva, N. P, ISO/TC 61/SC 14 "Plastics and Environment" / WG 4 „Microplastics“ (DIN Expert)

Ivleva, N. P, DIN-Normenausschuss NA 054-01-06 AA „Kunststoffe und Umweltaspekte“

Ivleva, N. P, NA 057 DIN-Normenausschuss „Lebensmittel und landwirtschaftliche Produkte“, NA 057-08-05 AA Arbeitsausschuss „Bestimmung von Mikroplastik in Lebensmitteln“

Seidel, M., Member of the Scientific Committees at the European BioSensor Symposium

Seidel, M., Member of the working group „Messen und Bewerten von Legionellen“ (NA 134-03-07-09 UA) bei der Kommission Reinhaltung der Luft im VDI und DIN

Seidel, M., Member of the working group „Bioaerosole und biologische Agenzien – Luftgetragene Mikroorganismen und Viren“ (NA 134-03-07-04 UA) bei der Kommission Reinhaltung der Luft im VDI und DIN

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

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

Theses

PhD Theses

MSc Wasserbau Sayed Amininejad: Nanoparticles and light - Characterization of dynamic changes to nanoparticle surfaces.

MSc Chem. David Bauer: Application of Raman Microscopy For a Rapid Antibiotic Susceptibility Test and the Investigation of Dormant Mycobacteria.

MSc Chem. Elisabeth von der Esch: The Automation and Validation of a Morphological and Chemical Quantification Procedure for Microplastic Fragments using Raman Microspectroscopy.

Dr. Lisa Katharina Morgane Göpfert, MSc Chem.: Rapid methods for the analysis of pathogens, antibiotic resistance genes, and microplastic-associated bacteria in water samples.

Dr. Sandra Hess, MSc Biochem.: Rapid concentration and detection methods for enteric viruses in water.

Dr. Bernhard Köhl, MSc Geol.: Scalings im Thermalwasserkreislauf.

Dr. Anne Heidi Landmesser, MSc Tox.: Biomarker-based dosimetry for e-cigarette users using stable-isotope labeled precursors and MS/MS analysis.

MSc Chem. Verena Meyer: Etablierung von regenerierbaren Chemilumineszenz-Mikroarray-basierten Immuno- und Rezeptor-Assays für den Nachweis von Antibiotika in flüssigen (Umwelt-) Proben.

Dr. Katharina Sollweck, MSc Biol.: Flow-based chemiluminescence bioassays for rapid screening of fungi, antibiotic resistant bacteria and diclofenac.

Dr. Fengchao Sun, MSc Hydrogeol.: Insights from isotope fractionation on limitations of micropollutant biodegradation—evaluating mass-transfer limitation and biodegradation in a bench-scale aquifer.

Dr. Yanwei Wang, MSc: Integration of 3D microfluidic platform with gold nanoparticle-catalyzed chemiluminescence analysis system.

M.Sc. Theses

Michael Alexander Becker, MSc Chem.: Entwicklung einer Extraktionsmethode für Non-Target Screening in Sedimenten und Schwebstoffen aus Flüssen.

Aoife Canavan, MSc Chem.: Quartz Crystal Microbalance as a Tool for Online Monitoring of Natural Organic Matter during Clean-Up of Organic Extracts.

BSc Lucas Hirschberger: Process Analytics with Raman and Fluorescence Spectroscopy.

BSc Sonja Hoffmann: Investigation of Functionalized Porous Aluminium Oxide as Sensitive Layer for Electronical Gas Detection.

Maximilian Huber, MSc Chem.: Towards the analysis of environmental samples by the online-coupled FFF-Raman microspectroscopy setup.

Jonathan Koch, M.Sc. Biochem.: Screening and Optimisation of primers for isothermal nucleic acid amplification test for rapid quantification of *Legionella pneumophila.*

Yiao Liang, M.Sc. Chemieingenieurwesen: Development of immunomagnetic beads for continuous monitoring of algae toxin in surface water.

BSc Felix Ludwig: Laser Desorption Mass Spectrometry for the Analysis of Atmospheric Nanoparticles.

BSc Kevin Maier: Laser and Thermal Desorption Mass Spectrometry for the Analysis of Atmospheric Particles.

Sandra Paßreiter, M.Sc. Chem.: Development and Optimization of Flow-Based Chemiluminescence Microarray Immunoassays for SARS-CoV-2 Serosurveillance.

Julian Trommler, M.Sc.: Immobilization of bacteriophages on monolithic affinity columns for the detection of *Escherichia coli*.

Julian Weng, MSc Chem.: Raman microspectroscopy for nondestructive analysis of microbial plastic degradation.

Justus Wettich, M.Sc. Physik: Entwicklung einer automatischen Auswertung von LegioTyper-Messdaten unter Verwendung maschineller Lernmethoden.

B.Sc. Theses

Christina Krahulikova: Impact of Riverine Organic Matrix on Compound-Specific Stable Isotope Analysis.

Kevin Li: Simultaneous Fluorescence and Absorption Analysis of Model Samples and Evaluation using Multiple Linear Regression.

Ines Mazurek: Entwicklung und Testung eines internen Standards für die magnetische Durchflusszytometrie.

Sarah Prakesch: Use of Aliivibrio Fischeri as Non-target Toxicity Test.

Peter Schmöller: Layer-by-Layer-Deposition und magnetischen Messungen im Fluss.

Nina Weidlein: Thermal Desorption and Mass Spectrometry for Atmospheric Nanoparticle Characterisation.

Teaching

Winter Semester 2020/2021

Analytische Chemie I, Instrumentelle Analytik

240242322 Geo-Umwelt LMU (BSc Geo.) M. Elsner

Chemische Analytik II - Organische Spurenanalytik für Geowissenschaftler

820486258 Geo-Umwelt LMU (BSc Geo.) M. Elsner

Wasserchemie 1

820005191 Geo-Umwelt LMU (BSc Geo.) M. Elsner

Angewandte Wasserchemie

0000005206 Chemistry (MSc Hydrogeo.) M. Elsner, R. Bakour

Chemische Analytik II – Organische Spurenanalytik für Geowissenschaftler

820486258Geo-Umwelt LMU (BSc Geo.) M. Elsner

Current Research in the Instrumental Analysis of Trace Components 1 (Practica)

0000001973 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Current Research in the Instrumental Analysis of Trace Components 1 (Lecture)

0000002469 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Environmental Chemistry

0000001972 Chemistry (MSc Env. Eng.) M. Elsner, R. Bakour

Fortgeschrittene analytische Verfahren

0000004763 Chemistry (BSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Hydrochemisches Praktikum

820678299 Hydrology (MSc) R. Bakour, C. Haisch

Hydrochemisches Praktikum für Geologen

0000003397 Hydrology (MSc Geo.) R. Bakour, C. Haisch

Hydrogeologisches, hydrochemisches und umweltanalytisches Seminar

240037914 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Spurenanalytik für Biochemiker

0000005683 Biochemistry (BSc) M. Seidel, N. P. Ivleva

Instrumentelle Methoden der Anorganischen Chemie

(CH3000b) 0000002336 (MSc Chem.) M. Elsner, N. P. Ivleva…

Lab Rotation Analytical Chemistry 1 (CH3124)

0000002910 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Lab Rotation Analytical Chemistry 2 (CH3125)

0000002932 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Seminar Institut für Wasserchemie

0000004167 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Summer Semester 2021

Automatisierung und Visualisierung von Laborprozessen und Daten

0000004577 Chemistry (MSc Chem.) M. Elsner, N. P. Ivleva, E. v. d. Esch

Biochemische Analytik

0000001651 Weihenstephan (BSc Bio.) M. Seidel

Biochemische und molekularbiologische Verfahren in der Umweltanalytik II – Enzymatische Verfahren, DNA Sonden

820032502 M. Seidel

Spurenanalytik für Studierende der Biochemie

0000005683 Garching (BSc Biochem.) M. Seidel, N.P. Ivleva

Case Studies in Analytical and Environmental Chemistry

0000002532 Chemistry (MSc Chem.) M. Elsner, R. Bakour

Aerosole: Bedeutung, Vorkommen und deren Charakterisierung

0000005602 Chemistry C. Haisch, R. Nießner

Hydrogeologisches, hydrochemisches und umweltanalytisches Seminar

240037914 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Instrumentelle Methoden der Anorganischen Chemie (CH3000b)

0000002336 (MSc Chem.) M. Elsner, N. P. Ivleva

Lab Rotation Analytical Chemistry 1 (CH3124)

0000002910 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Lab Rotation Analytical Chemistry 2 (CH3125)

0000002932 Chemistry (MSc Chem.) M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Physikalisch-chemische Aerosolcharakterisierung

0500003556 Chemistry C. Haisch

Physikalisch-chemische Aerosolcharakterisierung Blockpraktikum

0500001944 Chemistry C. Haisch

Praktikum Umweltmesstechnik

820176417 Chemistry C. Haisch

Seminar Institut für Wasserchemie

0500003454 Chemistry M. Elsner, C. Haisch, N. P. Ivleva, M. Seidel

Staff

Post Docs

Dr. Benjamin Heckel
Dr. Aileen Melsbach

Technical & Administrative Staff

Felix Antritter
Birgit Apel†
Christine Beese
Roland Hoppe
Susanne Mahler
Dipl.-Ing. Marco Matt
Cornelia Popp
Hatice Poyraz
Christine Benning
Sebastian Wiesemann

PhD Students

MSc Phys. Emilio Ambra
MSc Chem. Andreas Auernhammer
MSc Chem. David Bauer
MSc Lemi. Irina Beer
MSc Environ. Sci. Lihong Chai
MSc Geo. David Glöckler
MSc Chem. Lena Heining
MSc Chem. Lucas Hirschberger
MSc Chem. Maximilian Huber
MSc Chem. Oliver Jacob
MSc Chem. Julia Klüpfel
MSc Chem. Eva Krois
MSc Tox. Aileen Melsbach
Dipl.-Phys. Peter Menzenbach
Dipl.-Biochem. Oleksii Morgaienko
MSc Chem. Kara Müller
MSc Chem. Julia Neumair
MSc Chem. Leonhard Prechtl
MSc Chem. Christian Schwaferts
MSc Biochem. Gerhard Schwaiger
MSc Biol. Katharina Sollweck
MSc Chem. Philipp Streich
MSc Chem. Armela Tafa
MSc Chem. Christopher Wabnitz
MSc Chem. Yanwei Wang

External PhD Students

MSc Chem. Franziska Adler (Stadtwerke München)
MSc Chem. Jessica Beyerl (LMU-Tropeninstitut)
MSc Chem Leopolf Daum (TUM, Heinz-Nixdorf-Lehrstuhl für Biomedizinische Elektronik)
MSc Chem. Matthias Edelmann (TUM, Lebensmittelchem. u. molekulare Sensorik)
MSc Chem. Melina Grasmeier (Klinikum rechts der Isar)

MSc Chem. Amelie Hohensee (LMU-Tropeninstitut)
MSc Tox. Anne Landmesser (ABF GmbH München)
MSc Chem. Maria Lanzinger (BMW)
MSc Chem. Janine Potreck (Klinikum rechts der Isar)
MSc Chem. Markus Weber (Plasmion GmbH Augsburg)

Master Students

BSc Chem. Aoife Canavan
BSc BWL-Chem. Jonas Flechtner
BSc Chem. Lucas Hirschberger
BSc Chem. Sonja Hoffmann (Fraunhofer EMFT)
BSc Chem. Maximilian Huber
BSc Biochem. Jonathan Koch
BSc Bioanal. Marie Kröger
BSc Chem. Eva Krois
BSc Chem.-Ing Yiao Liang
BSc Chem. Felix Ludwig
BSc Chem. Kevin Maier
BSc Chem. Sandra Paßreiter
BSc Tech & MMG Julian Trommler
BSc Chem. Julian Weng

External Master Students

BSc Chem. Alexander Thomas (BMW)
BSc Physik Justus Wettich (GWK)

Bachelor Students

Kristina Krahulikova
Kevin Li
Ines Mazurek
Sahra Prakesch
Peter Schmöller
Nina Weidlein

Guests

Dr. Jamila Boudaden (Fraunhofer EMFT)
MSc Camilla Marasca (Uni Bologna, PhD)
MSc Corinna Winkler (Klinikum rechts der Isar)
Dr. Jan-Christoph Wolf (Plasmion GmbH)
Dr. Silvia Würstle (Klinikum rechts der Isar)
Dr. Klaus Wutz (Plasmion GmbH)

Student Assistants

Ayesha Navaid Anwar
Nico Chrisam
Beatriz von der Esch
Charlotte Heinritz

Maximilian Huber
Alexander Kohles
Kevin Maier
Alejandro Ramirez Pinero
Nina Weidlein
Julian Weng

Equipment

Aerosol Research

1 Aerosol chamber (1 m^3)

1 Aerosol flow tube (10 L)

1 Ozone analyzer (UV absorption)

1 NO/NO_2 analyzer (Chemiluminescence)

1 Aerodynamic particle sizers (0.5-25 µm)

1 Laser Aerosol Spectrometer (size range 90 nm -7.5 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)

3 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 AVL Micro Soot Sensor with dilution unit

2 FT/IR gas analyzers

Microarray Technology

1 Chemiluminescence Microarray Reader, MCR 3, GWK Präzisionstechnik GmbH

3 Chemiluminescence Microarray Reader, MCR R, GWK Präzisionstechnik GmbH

1 Ink-Jet Microdispenser, SciFlexarrayer S1, Scienion

2 Contact Microarrayer, BioOdyssee Caligrapher, BioRad

2 Cutting Plotter, Graphtec CE6000-40

Microbiology

1 Flow Cytometer, CyFlow Cube 6, Sysmex Partec GmbH

1 qPCR, qTower^{3}G qPCR, Analytik Jena GmbH

1 DNA extractor, InnuPure C16, Analytik Jena GmbH

1 Bead Beater Homogenizer, MP Biomedicals

1 IMS / Flow Cytometer for *Legionella pneumophila*, rqmicro AG

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

2 Clean Benches

1 Bioaerosol Chamber

2 Microbiological Incubator, Binder

1 Temperature Controlled Shaking Incubator

1 Autoclave, Certoclav

1 Autoclave, SHP Steriltechnik

1 Cyclone Impinger Coriolis µ, Bertin

1 Munich Microorganism Concentrator, MMC 3

1 Monolithic Affinity Filtration Unit

Standard Lab Equipment

1 Lyophilizer, Alpha 1-4 LSC, Christ

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

1 Centrifuge, Eppendorf 5804 R

2 Fluorescence Spectrometer LS 50, Perkin Elmer

1 UV-Vis Spectrometer, Perkin Elmer

Bioanalytics and Microanalytical System Group

1 Cooled Centrifuge, Universal 320R, Hettich

1 Climatic Chamber, Binder

4 Drying Cabinets, Memmert

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

1 Photometric ELISA Reader, Biotek

1 96-channel Washer, Biotek

1 Turbidometer, WTW GmbH

1 Nanophotometer, Implen GmbH

1 -80 °C Freezer

Chromatography, Mass Spectrometry and Particle Separation

2 GC-IRMS (Isotope Ratio Mass Spectrometer) Instruments

2 GCs with FID and ECD

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

1 MS, Thermo Fisher LTQ

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
1 LC system, ECONO
1 Preparative HPLC
Elemental Analysis
1 Flame-Photometer, BWB Technologies
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
several diode lasers (600-1670 nm; up to 2 W CW)
several Quantum Cascade Laser systems
3 Optical parameter oscillator (410 nm-2.1 µm)

Optoelectronics/Spectrometer

3 Echelle spectrometer
1 FTIR-Spectrometer, Thermo Scientific Nicolet 6700
1 Fluorescence spectrometer, Perkin Elmer LS-50
1 Fluorescence spectrometer, Shimadzu RF 6000
1 UV/VIS spectrometer, analytic jena Specord 250 plus
1 UV/VIS spectrometer, analytic jena Spekol 1500
4 Digital storage oscilloscopes (400 MHz, 500 MHz)
1 Wavemeter

Microscopy

2 Laser Raman microscope, WITec *alpha300R* (532/633 nm)
1 Laser Raman microscope, WITec *apyron* (532/785 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)
1 SEM/EDX system, Zeiss Gemini

Sum Parameters

2 Coulostat for C quantification, Coulomat 702
1 DOC analyser, UNOR 6 N
1 TOC analyser, Shimadzu TOC-L