



Annual Report 2014



Measurement campaign for siloxane and sulfur detection in biogas at the Garching wastewater treatment plant

Institute of Hydrochemistry and Chemical Balneology
Chair for Analytical Chemistry
Technische Universität München
Marchioninstr. 17
D-81377 München
<http://www.ws.chemie.tu-muenchen.de>

Editor: Dr. Thomas Baumann

Editorial

Dear coworkers, friends & colleagues!

Germany has a long history in Analytical Chemistry, but only a few of you may know that the founder of the German Analytical Chemistry as a discipline, Carl Remigius Fresenius, started research and teaching around 1830 because the medical treatment of patients by warm mineral spring water called for an in-depth analysis of the chemical composition. In 1861, more than 150 years ago, the combination of water chemistry and the need for quantitative and qualitative characterization of mineral water led to nascence of the German Analytical Chemistry and to the foundation of "Fresenius' Zeitschrift für Analytische Chemie", up to now very active and known as Analytical & Bioanalytical Chemistry.

The Institute of Hydrochemistry, IWC for short, as well has long standing experience and expertise in Analytical Chemistry. Already under the auspices of my predecessor, Prof. K.-E. Quentin, it was the leading German Institute for Hydrochemistry for decades and also responsible for the outline of numerous standard guidelines for water analysis. I feel honoured to act as Head of the Institute and Chair of Analytical Chemistry for more than 25 years.

As you will notice in this report, we are still full in line with this long lasting tradition. Our hydrogeological branch, headed by PD Baumann, is deeply involved in research within and around geothermal water wells. This green technology is thought to be very safe and sustainable. But you may imagine what will happen with hot mineral water, fully saturated with minerals and gases, when it is pumped from 3000 m below surface level to the facilities at ground level, where reduced pressure and lowered temperatures disrupt all dissolved matter equilibria, causing corrosion, scalings and failures all along thermal water pathway. A costly experience numerous facilities had to make.

On the other hand, clean water is only provided by nature, as long as the (vertical) water cycle is working well. There is a high risk of contamination, already within clouds, where liquid water is "born". Thus, humans can only rely on a safe and adequate natural ground water resources if the percolation through soil and aquifers, where ion exchange, sorption and decay take place is still working as a cleaning process. This process is heavily challenged not only by polar contaminants and viruses. Therefore, to maintain highest quality of this recycled natural product – water – we need the best technologies to observe its chemical and microbiological status. This is the reason, why water chemistry and analytical chemistry do so well together !

The IWC has also become a worldwide renowned centre for advanced analytical technologies, laser- or receptor-based, you name it. The laser group, headed by PD Haisch, is successful with quantum cascade laser technology to measure N₂O emissions above and within a sewage water treatment plant online. The aim is an optimized control of climate relevant emissions. Nanoparticles used to tag antibodies allow extreme sensitive detection of toxins, as it was developed in the group of Prof. Knopp.



The chase for viruses within surface water requires enormous enrichment from about 100 m³ down to 1 mL (!), in order to apply microarray PCR in a highly parallel fashion. This is a specialty of the research group of PD Seidel.

It seems that 2014 was the year of micro plastics. Tiny pieces and fragments of these ubiquitous products became identified almost everywhere. We contributed to the detection and identification with a refined sampling procedure and device, the Munich Plastic Sediment Separator, and an excellent identification protocol, developed by Dr. Ivleva in our Raman Microspectroscopy Centre, which uses Raman microspectroscopy to reduce the ambiguity of conventional optical detection methods and to extend the detectable range of particles orders of magnitude to smaller particles. News media were full of it !

In essence, it seems that the Institute and it's scientists are in good tradition with Carl Remigius Fresenius. For this, I would like to thank all my coworkers, especially the many PhD students we still have, and the permanent staff of IWC.

Reinhard Niessner

Hydrogeology (PD Dr. T. Baumann)

Effects of Physical and Chemical Surface Heterogeneity on the Transport of Engineered Inorganic Nanoparticles

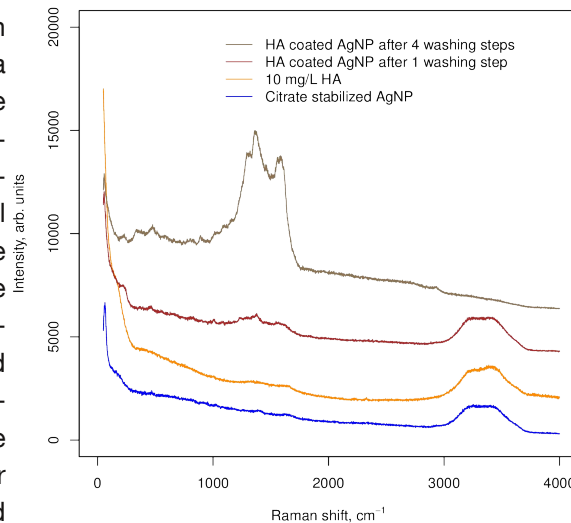
Funding: DFG (Deutsche Forschungsgemeinschaft)

Cooperation: DFG Research Unit InterNANO (FOR1536)

The widespread use of engineered inorganic nanoparticles (EINP) leads to a growing risk for an unintended release into the environment. Despite a good characterization of EINP with regard to their function scale and the application areas, there is still a gap of knowledge concerning their behaviour in the different environmental compartments. Due to their high surface to volume ratio, surface properties and existence or development of a coating are of high importance for their stability and transport behaviour. However, analytical methods to investigate organic coatings on nanoparticles in aqueous media are scarce. We used Raman microspectroscopy in combination with surface-enhanced Raman scattering (SERS) to investigate humic acid coatings on silver nanoparticles under environmentally relevant conditions and in real world samples. This setup is more challenging than previous mechanistic studies using SERS to characterize the humic acids in tailored settings where only one type of organic matter is present and the

concentrations of the nanoparticles can be easily adjusted to the experimental needs. SERS offers the unique opportunity to work with little sample preparation directly with

liquid samples, thus significantly reducing artefacts. SERS spectra of different natural organic matter brought into contact with silver nanoparticles indicate humic acid in close proximity to the nanoparticles. This coating was also present after several washing steps of centrifugation and re-suspension in de-ionized water and after an increase of



SERS spectra of AgNP coated with humic substances, citrate stabilized AgNP and the dissolved humic substances

ionic strength. TEM images and AF⁴ measurements indicate a coating thickness of only a few nanometers. To simulate more natural conditions, Ag NP were aged in river water from the river Rhine and soil solution obtained from a stagnic cambisol from a floodplain area of the river Rhine. SERS measurements showed peaks typical for humic substances indicating a humic coating around the nanoparticles

M. Kühn

Quantification of Heat Mining in the Bavarian Molasse Basin

Funding: BMU (Federal Ministry for the Environment, Nature Conservation and Nuclear Safety)

Cooperation: IEP GmbH, Pullach; Erdwerk GmbH, Munich; Aquasoil GmbH, Berlin

Geothermal energy is a key technology for the transition from fossil resources to renewable energy. The Bavarian Molasse Basin offers unique hydrogeological conditions for district heating and power generation. With 15 plants operating and another dozen in construction or planning, exploration is highly successful. However, detailed knowledge about the processes occurring in the aquifer which is crucial to run geothermal facilities is scarce.

After more than 10 years of operation there is a good record of the hydraulics and the hydrochemistry at the production well, including numerous data

from pump failures and the development of precipitates. The injection well and its surrounding, however, is usually a black box which is not readily accessible. Here, not even the temperatures in the immediate vicinity have been measured. Nevertheless, the performance of the aquifer near the injection well controls the long-term operation of the geothermal system.

Thanks to an extension of the Pullach geothermal facility with a third well in 2011 there was a unique opportunity to produce water from a former injection well after

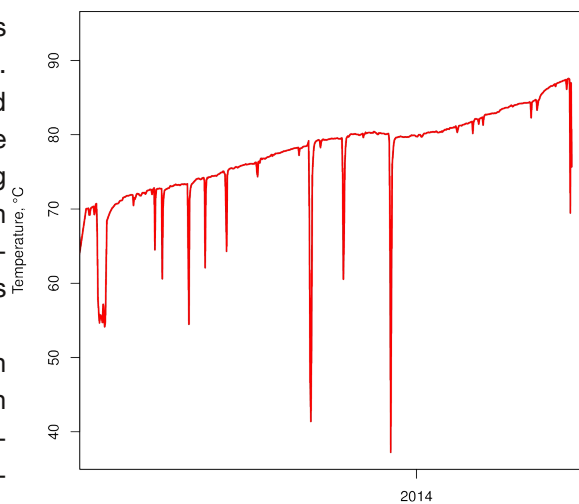
5 years of operation. Since the start of the production from this well in 2012, we collected an extensive data set of hydraulic, thermal and hydrochemical data.

Within the first two years after reverting the flow direction and at a production rate of 20 L/s, which is significantly lower

than the injection rate of up to 35 L/s, the temperature at the well head increased with a rate of 10 K/a. These temperatures were compared with predictions from the initial heat mining model, which was then refined. From the data it was immediately obvious that a homogeneous treatment of the Malm aquifer is not

applicable. Instead a heterogeneous flow regime has to be assumed to account for the fast initial increase of the temperatures which is caused by a higher effective exchange area. The results suggest that the regeneration time of the cooled reservoir in this setting is not too much longer than the injection period. Heat energy is primarily supplied by the water drawn to the well and heat conduction in low flow zones. This has to be taken into account when designing future facilities with more wells.

M. Lafogler



Temperatures at the well head of the former injection well since the start of production

Minimizing Risks for Geothermal Power Plants

Funding: BMU (Federal Ministry for the Environment, Nature Conservation and Nuclear Safety)

Cooperation: SWM Services GmbH, Munich

Scalings in the thermal water system are a serious problem especially for the "over 100s", that is facilities with production rates of about or more than 100 L/s and temperatures over 100 °C. Here, even small changes of the pressure lead to degassing and the formation of precipitates. Scalings start at the pump and continue throughout the system. Even at the injection wells serious precipitates occur when the pressure is dropping below the bubble point of the dissolved gases.

Scalings limit the operation of the geothermal fa-

cility and are risky and costly. One out of ten changes of the pump is problematic, sometimes with a complete loss of the pump. Furthermore the tubings, i. e. their threads, are not designed for permanent exchanges. In the ground level facilities, scalings reduce the efficiency of the heat exchange, this has not yet been a major problem only because the facilities do not operate at full throttle yet.

It has been shown that the rate of precipitation at the well head is depending mostly on the produced volume while the scalings above the pump not only indicate a highly dynamic system but are also depending on the type of pump used. It seems that the hydraulic design of the pump's interior is

crucial and a target for optimization. The current use of filter systems in the ground level facilities seems questionable. The filter efficiently remove particles which is necessary after restarting the production. However, small particles act as condensation nuclei

and thus might reduce precipitation at the tubings.

Monitoring of the gas loading and gas composition revealed a short-term variance of 10 %, whereas changes of 25 % over several weeks and more than 50 % over the years.

Today it is not yet

clear, whether this is due to technical reasons (pumping rate, pressure gradients) or a manifestation of varying concentrations in the water. Either way, as the gas loading strongly affects the formation of precipitates, the pressure in the system has to be set to higher levels or dynamically adjusted. The monitoring of the gas composition also was able to indicate a failure of the pressure holding system. Video control of degassing at ground-level might provide quick access to the efficiency of the pressure holding system.

In order to minimize risks, one has to invest into dedicated monitoring tools for the gas composition, at least for the moment.

M. Herbrich



Scalings inside of the stand pipes

High-Temperature-Aquifer Storage

Funding: BMW (BayINVENT)

Cooperation: TUM Hydrogeology; Erdwerk GmbH, Munich; Aquasoil GmbH, Berlin

Combined heat and power generation (CHP) is highly efficient because excess heat is used for heating and/or process energy. However, the demand of heat energy is highly variable throughout the year while the demand of electrical energy is rather constant. It seems economically highly beneficial and ecologically sound for municipalities and large power consumers such as manufacturing plants to store excess heat in groundwater aquifers and to recuperate this energy

at times of higher demand. Apart from the hydrogeological conditions, high transmissivity and favorable pressure gradients, the hydrochemical conditions are crucial for long-term operation.

After a year of planning, construction, and the successful drilling of a research well to 495 m below surface level the first large scale heat storage test in the Malm aquifer was finished just before Christmas. About 4 TJ of heat energy were injected into the Malm aquifer using hot water in five distinct pulses. The temperatures started at 60 °C and went up to 110 °C and the injection and production rates were 15 L/s. With each pulse conservative and reactive tracers were

injected to gain information about the hydraulic conditions. CO₂ was added to the water before heating to maintain equilibrium conditions for the dissolved carbonates. Later dismantling of the heat exchangers showed no scalings at all, proving the efficiency of the CO₂ addition.

Energy recovery during the first pulses was above 35% and rising. As a side effect of the extremely good hydraulic conditions, the research well was flowing freely with 15 L/s, there was significant

mixing of the injected water with formation waters during production. This was unambiguously quantified using the different chemical composition of the injected water and the formation water. There was little dissolution of carbonates due to a change of the saturation index of calcite as the water was cooling down in the aquifer.

The recovery rates for the tracers were well above 60% depending on the type of tracer. Complementary laboratory experiments showed different transport velocities in column tests which were related to different sorption behaviour.

M. Ueckert



Replenishment of resources during the heat storage test

Bioanalytics (Apl. Prof. Dr. D. Knopp)

Microbial Fuel Cell - Development and Application as Biochemical Oxygen Demand Sensor

Funding: IWC

Cooperation: Max von Pettenkofer-Institut, LMU, Prof. Dr. S. Schubert

The Biochemical Oxygen Demand (BOD) is a widely used criterion for water quality assessment that provides information about the organic load in water and wastewater. However, the conventional analytical method for the determination of the BOD is time-consuming and therefore, new methods for a continuous water quality monitoring would be preferable. In this study a microbial fuel cell (MFC) was tested as an option.

All measurements were operated in continuous flow. When the MFC containing, e.g., *Shewanella putrefaciens* in the anode chamber, was fed with Lysogen Broth-medium (LB-medium) a maximum signal value of 1070 μA was recorded. Supplying the MFC with different concentrated LB-media led to a change in the electric current. A decrease of the current was observed following the gradual dilution of the medium. When *Shewanella putrefaciens* was adapted to conditions where only few nutrients were present, higher sensitivities were obtained. On this account, the effect of different

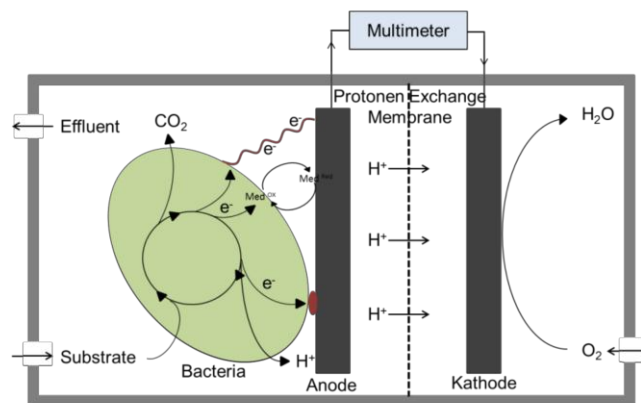
substrates such as glucose or Sodium-acetate on the current could be observed when *Shewanella putrefaciens* was adapted to low-nutrients condition.

For possible application of the MFC to

real samples, wastewater was flushed through the MFC containing different populations of microorganisms in the sewage sludge in the anode chamber. A current was generated by exoelectrogenic strains like *Aeromonas hydrophila*

and *Klebsiella pneumonia*, which could be identified by MALDI-TOF-MS. Because of the toxic action of silver nanoparticles and carbon nanotubes, the microbial activity is inhibited and thus the power output of the MFC decreased. Therefore, the MFC could also serve as an early toxicity warning device.

C. Hartmann, A.-C. Neumann

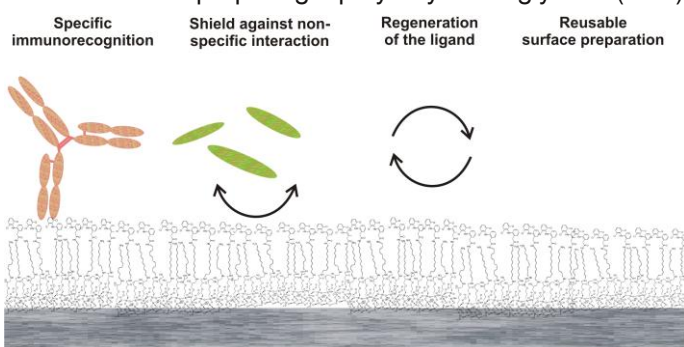


Schematic setting of a MFC

Nanoscaled Architectures for Highly Sensitive Biosensing of Small Molecules

Funding: DFG (Deutsche Forschungsgemeinschaft)/ANR (Agence Nationale de la Recherche)
Cooperation: Université Pierre et Marie Curie, Paris, France, Prof. Dr. S. Boujday, Prof. Dr. A. Proust, Prof. Dr. C.-M. Pradier

In this project, we focus on the mechanism of molecular recognition at the nanoscale for the detection of priority pollutants in surface water. For reliable measurements, a strategy for preparing polyethylene glycol (PEG)



Properties of a surface preparation for haptens immunosensing

coatings for subsequent haptens immobilization on glass-type chip surfaces is characterized step by step. Two surfaces were investigated, silicon wafers and glass slides and were applied to the competitive detection of a pharmaceutical target, diclofenac. First, surfaces were thoroughly cleaned and a silane layer with terminal epoxy groups was created using 3-glycidyloxypropyltrimethoxysilane (GOPTS). GOPTS reaction with diamino - poly(ethylene glycol) (DAPEG) led to a layer with terminal amino groups. The diclofenac was attached via its carboxylic acid group.

In the laboratory of our French project partners, different methods for surface analysis were used to investigate the resulting surface structure. Attenuated Total

Reflection (ATR) was used to collect FT-IR spectra to monitor the change of the chemical composition. Contact angle measurements showed that the hydrophilicity is equal for both surfaces (Si and glass slide) after the PEG coating. Atomic force microscopy (AFM) images showed a smooth layer at this stage. These examinations indicate that the PEG serves as a shielding layer on both substrates for interface interactions with the antibodies in aqueous solution. Moreover, X-Ray Photoelectron Spectroscopy (XPS) was used to estimate the layer thickness after each preparation step. In this way, the monolayer formation of the silane grafting and PEG coating can be shown. The analyzed surface chemistry was applied to assess the reusability of the recognition structure on the surface by a quartz sensor chip for Quartz Crystal Microbalance with dissipation (QCM-D) measurements with polyclonal anti-diclofenac serum. The surface was regenerable and highly stable for repeated measurements on the same QCM-D electrode at different days. Finally, the reusability was shown for a microarray of diclofenac in 30 measurement cycles using an automated flow-through immunoassay with chemiluminescence (CL) readout. In the aftermath to this analysis, we will construct a multiplex method with CL detection for different priority pollutants in surface water based on monoclonal antibodies.

M. Hübner

Investigation of paratope-epitope interactions of anti-PAH antibodies

Funding: Hanns-Seidel-Stiftung, IWC

Cooperation: Department of Chemistry, Physical Chemistry, Universität Potsdam (Prof. Dr. M. Kumke) and Chair of Biological Chemistry, TU München, Prof. Dr. A. Skerra)

Polycyclic aromatic hydrocarbons (PAHs) are a large group of ubiquitous environmental pollutants. They are built up of at least two condensed benzene rings that form a linear, angular or ring-shaped arrangement. During the past years, one of our main efforts was focused on the generation of highly affine antibodies against PAH compounds for their use as selective receptors in different immunoassay formats.

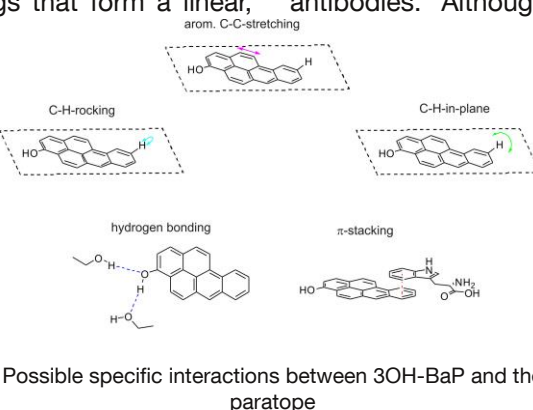
The understanding of the physicochemical interactions between an antigen and the paratope of the formed antibody is crucial for any efforts of genetic modification in order to improve the antibodies' binding characteristics. In this project, fluorescence line narrowing spectroscopy (FLNS) (collaboration with Prof. Kumke) and X-ray crystallographic analysis (collaboration with Prof. Skerra) were used to investigate the immune complex formed between 3-OH-benzo[a]pyrene (3OH-BaP) and different murine and recombinant antibodies. FLNS is especially valuable for hydrophobic haptens, for which formation of antibody-hapten complex crystals is extremely difficult. Based on IR and Raman data, fluorescence bands were correlated with respective ground state vibrations of the hapten and this information

used to characterize the molecular interactions between 3OH-BaP and a variety of different solvents (as model systems) and antibodies. Although the analyte was the same for all antibodies investigated, different binding interactions could be identified from FLN spectra on the bases of structural flexibility and conformational multiplicity of the paratopes. In general, van-

der-Waals interactions were identified as a major class of binding interactions. In addition, π -stacking was observed.

For production of crystals suitable for X-ray scattering, in contrast to our earlier work, Fab fragments of the murine antibody 22F12 have been produced by recombinant techniques, established at Prof. Skerra's laboratory. The Fab properties have been optimized for crystallization and the produced Fabs were characterized for their affinity towards benzo[a]pyrene (BaP) using ELISA and Surface Plasmon Resonance spectroscopy (SPR). Finally, crystallization was successful and X-ray crystallographic analysis performed.

M. Pschenitza



Depletion of Algal Toxin-Contaminated Water Using Selective Biofilters Based on Plant-Produced Antibodies (Plantibodies)

Funding: DFG (Deutsche Forschungsgemeinschaft)/FWF (Fond zur Förderung der wissenschaftlichen Forschung)

Cooperation: University of Natural Resources and Life Sciences (BOKU), Vienna, Austria, Prof. Dr. E. Stoeger

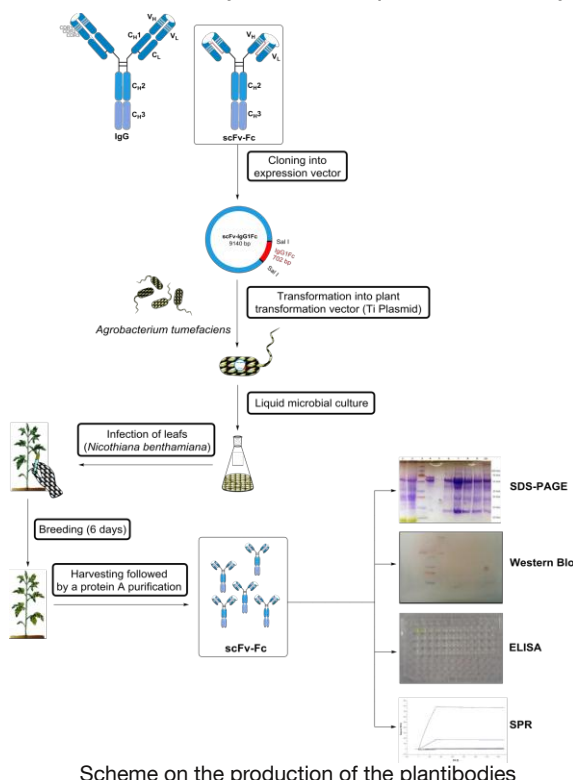
Cyanobacteria which can be found in almost every terrestrial and aquatic habitat produce a wide variety of unique secondary

The aim of the bilateral DFG/FWF-project is a genetic modification of special plants in order to express anti-MC-LR-antibodies, the so-called plantibodies. The idea is to develop efficient, selective and cost-efficient biofilter-based on the antibody-antigen-interaction for an *ex vivo* depletion of the toxin from water bodies.

First experiments focussed on using the existing mouse monoclonal antibody (MC10E7) in order to establish a reference for the plantibodies produced in the progress of the project. Several affinity columns were prepared using, e.g., the sol-gel technique or bead-based material to immobilize the antibodies. The binding capacities were estimated and compared with results already published in the literature. *Surface plasmon resonance* (SPR) measurements and indirect competitive *enzyme-linked immunosorbent* (ELISA) assays were carried out and showed high antibody affinity.

The plantibody production is operated by our partner by infection of *Nicotiana benthamiana* with *Agrobacterium tumefaciens* which carried a transformation vector with the sequences for the VL und VH region of the antibody MC10E7. After a cleaning step with protein A the received plantibodies are under testing by SPR and ELISA at the present.

A.-C. Neumann



metabolites – the toxins like anatoxin, saxitoxin, nodularin and microcystin. Microcystin-leucine-arginine (MC-LR) is the most toxic microcystin congener, destroying liver cells for example. The World Health Organization (WHO) recommends that the amount of free and cell bound MC-LR in drinking water is limited to 1 µg/L. Germany and the United States aspire this proposal.

Magnetic Bead-Based Colorimetric Immunoassay for Aflatoxin B1 Using Gold Nanoparticles

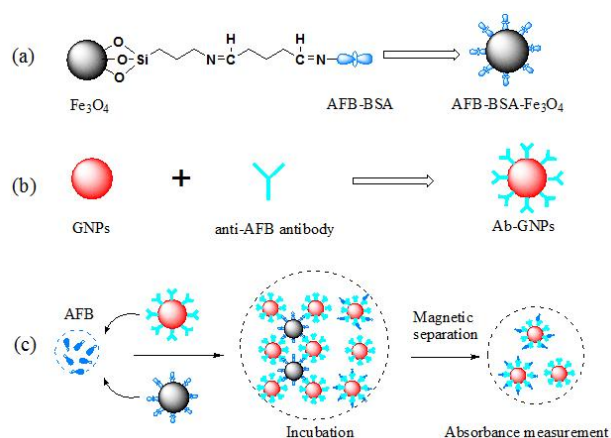
Funding: IWC, China Scholarship Council

Aflatoxins are highly toxic secondary metabolites produced by *Aspergillus flavus* and *Aspergillus parasiticus*. They may be present in a wide range of food and feed products. Among them the most hazardous aflatoxin B1 (AFB1, listed as Group I carcinogen) is usually predominant. Although different methods have been developed for AFB1 detection (HPLC, LC/MS, immunoassays, ...), fast and simple methods with high sensitivity and specificity are still desirable.

Optical biosensors coupled with nanotechnology provide a new approach to address this issue. Gold nanoparticles (GNPs) are probably the most attractive ones owing to their unique physical and chemical properties, such as easy preparation, simplicity of modification, superior biocompatibility and excellent optical properties. They are frequently employed as labels for different biological receptors. In addition, magnetic particles are extensively utilized in bioanalytical fields because they have a good biocompatibility and can be easily separated from reaction mixture with the aid of an external magnet.

A competitive colorimetric immunoassay for the detection of AFB1 has been established using biofunctionalized magnetic beads (MBs) and GNPs. AFB1-bovine serum albumin conjugates modified MBs (AFB1-BSA-Fe₃O₄) were employed as capture probe, which could specifically bind with GNP-labeled anti-AFB antibodies through immunoreaction, while such specific binding was competitively inhibited by the addition of AFB1. After magnetic separation, the

supernatant solution containing unbound GNPs was directly tested by UV-Vis spectroscopy. The absorption intensity was directly proportional to the AFB1 concentration. The influence of GNP size, incu-



Schematic illustration of the preparation of (a) AFB1-BSA-Fe₃O₄ MBs; (b) Ab-GNPs; and (c) principle of the competitive colorimetric immunoassay for AFB1 detection

bation time and pH was investigated in detail. After optimization AFB1 was quantified in a linear range from 20 to 800 ng/L, and a limit of detection of 12 ng/L. The recoveries for spiked maize samples ranged from 92.8% to 122.0%. Higher sensitivity could be achieved through signal amplification by coupling with the special catalytic properties of GNPs. For instance, GNPs could be used as seeds for catalytic deposition of silver or gold, followed by absorbance measurement. As another example, GNPs can catalyze the decolorization of organic dyes like rhodamine to generate significant colorimetric/fluorescent signal change. The effort to enhance assay sensitivity is underway.

X.Wang

Applied Laser Spectroscopy (PD Dr. C. Haisch)

Photoacoustic Spectroscopy for N₂O Analysis

Funding: IWC, International Graduate School of Science anring (IGSSE)

Cooperation: TUM, Chair of Urban Water Systems Engineering, Prof. Drewes

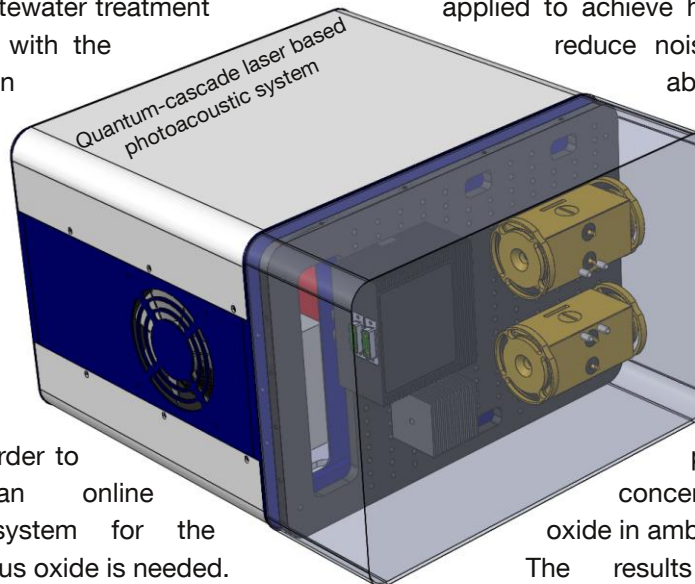
Trace gases like nitrous oxide (N₂O) increase the greenhouse effect and contribute to the depletion of the ozone layer. Anthropogenic sources of nitrous oxide are combustion engines and wastewater treatment plants. Together with the Chair of Urban Water Systems Engineering, we investigate the production of nitrous oxide in wastewater treatment plants under different process parameters. In order to do that, an online measurement system for the detection of nitrous oxide is needed.

Photoacoustic (PA) spectroscopy has proven to be a very sensitive method for gas analysis. The principle of PA spectroscopy is the conversion of absorbed light energy into acoustical waves which can be detected by means of a microphone. The robustness and simplicity of some PA techniques allow for in situ monitoring. Combined with a gas extraction technique like stripping or hollow fiber membranes it is possible to measure nitrous oxide in the liquid and in the gas phase with one system.

Our new PA system consists of a 4.5 μm quantum cascade laser (QCL), a PA cell, a microphone and an integrated lock-in amplifier. A 2f-wavelength modulation is applied to achieve high sensitivity and reduce noise caused by the absorption of the laser light at the cell wall or windows. With this mobile device it is possible to quantify nitrous oxide concentrations well below 300 ppb, which is the concentration of nitrous oxide in ambient air.

The results of the first measurements at the wastewater treatment plants were quite promising. A comparison of the QCL-PA system with a commercial N₂O sensor for liquid phase analysis showed a good correlation between both systems.

C. Berger



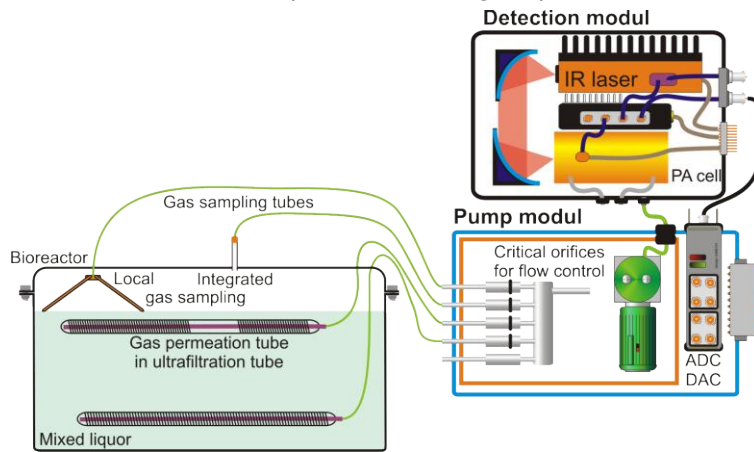
Sampling and Detection of N₂O in Wastewater Treatment Plants

Funding: International Graduate School of Science and Engineering (IGSSE)
 Cooperation: TUM, Chair of Urban Water Systems Engineering, Prof. Drewes

Nitrous oxide (N₂O) is a strong greenhouse gas with a significantly higher global warming potential than carbon dioxide. N₂O is produced by wastewater treatment plants during the biological nitrogen removal process. Due to the lack of comprehensive monitoring approaches there is limited data available to establish quantitative relationships between nitrous oxide emissions and process parameters of biological nitrogen conversions. The goals are to develop novel monitoring and control strategies for N₂O employing photoacoustic (PA) laser spectroscopy. That will enable a tight control of contemporary nitrogen removal processes as well as new ways in harvesting N₂O for enhanced energy recovery from waste streams.

A central role of the project is the development of an appropriate gas capture and conveyance system that will be connected to the PA-based monitoring device. Gas samples from multiple locations will be pumped continuously to the central

detection unit, while N₂O from different sampling ports will be measured sequentially. In addition, a novel sample device comprised of a gas permeable membrane, which is



Setup of the N₂O-monitoring system

submerged in the mixed liquor reactor, needs to be optimized to allow reliable gas phase measurements with the same PA unit. The task is to extract the solved N₂O gas from the

liquid phase. A highly selective membrane is needed, which is permeable to N₂O and impermeable to water. First experiments with different silicone membranes show promising results. Dimensions of the gas permeable membrane, as well as the gas flow have to be optimized, and potential aging due to biofilm growth will be investigated. Comparison of the PA-data with routine analytical methods (e.g. gas chromatography) is implemented.

The next step is the improvement of extraction efficiency and a test under real conditions.

K. Thaler

A Novel Plasmaspectroscopic System for Online Monitoring of Siloxanes in Biogas

Funding: IWC

Due to rising energy consumption and the drive to renewable energies, biogas is increasingly used as an energy source. The number of biogas plants has more than quadrupled in the last ten years in Germany. Depending on the energy utilization, determination of the composition and in some cases the removal of certain components is required.

Siloxanes are undesirable trace components, which can be found in varying concentrations in biogas from wastewater treatment. If these organosilicon compounds reach the combustion engines, they get oxidized to silicon oxide, which gets deposited in form of a white precipitate on parts of the engine. The crystalline SiO_2 can clog valves and cause overheating of motor parts, since the deposits act as a thermal insulator. Operators of landfills and sewage treatment plants must ensure that the siloxane concentration in combustion gas remains below the limits recommended by the engine manufacturer.

The goal of this project is the quantification of these compounds in biogas. A novel method based on plasma emission spectrometry is used. A gas discharge, generated by high voltage, serves as a plasma source. Its optical emission is detected by a spectrometer. By comparing several measuring cells, optical devices, and high-voltage sources, low detection limits are achieved.

A mobile measurement system has been built and tested under practical conditions. To improve the detection of siloxanes and avoid matrix effects a capture system has to be included. In this setup activated carbon is flushed with biogas. Afterwards the activated carbon is heated to approx. 300 °C. As a result siloxane desorbs and is analysed in the plasma. This process takes place in a metal tube which is heated contactless by an induction coil to ensure a fast cool down.

K. Thaler



Gas discharge plasma sensor as used for siloxane monitoring

Laser Photofragmentation for the Detection of Nitro-PAHs in Combustion Engine Exhaust

Funding: DFG (Deutsche Forschungsgemeinschaft)

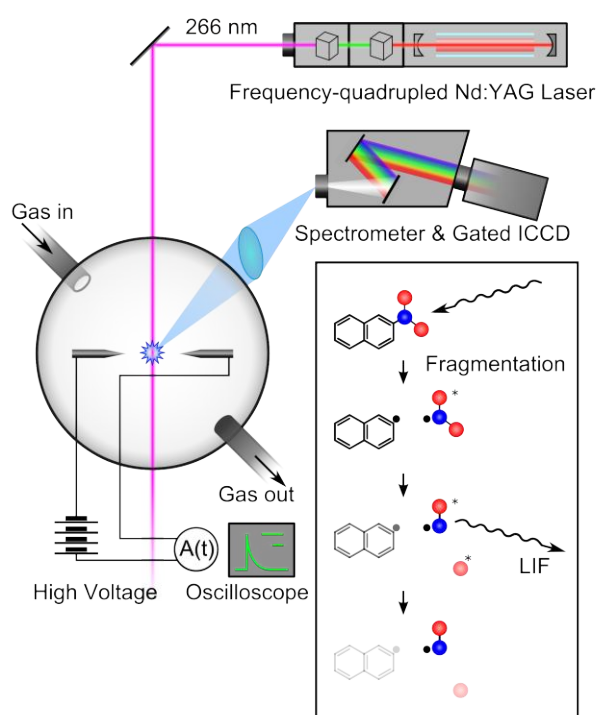
Nitrated polycyclic aromatic hydrocarbons (NPAHs), together with their parent compounds, PAHs, are probably the abiotic class of substances which is most harmful for human health, not only in the atmosphere, but in the total environment. More than a third of the mutagenic potential of ambient air is attributable to NPAHs.

Our aim is to employ photofragmentation (PF), the process of breaking chemical bonds through interaction with one or multiple photons, as a means to investigate NPAHs in the gas phase as well as adsorbed on aerosol particulate matter. High sensitivities in the low ppb or even ppt range for PF-based gas phase analysis can be achieved.

Different modalities can be distinguished, regarding the fragmentation mechanism and the way of fragment detection. Resonant fragmentation allows for a rather straightforward system set-up; a single laser pulse can be employed for fragmentation and photoionization. Depending on the photon energy employed, the fragments can be generated in an excited state, which relaxes by optical emission. This effect can be addressed as PF/fragment fluorescence, PF/spontaneous emission, or PF/prompt emission (PF/PE).

For nitrated aromatic compounds, a fragmentation process including elimination of nitrogen dioxide (NO_2) in an excited state and consecutive decay to excited atomic oxygen and excited nitric oxide (NO) is known. The generated NO molecules release their excitation energy optically. By using a

gated intensified CCD camera (ICCD), time-resolved broadband spectral analysis of the emitted fluorescent light should be possible. Simultaneously, photoionization can be detected by two high-voltage electrodes. The



Schematic of the experimental setup and fragmentation mechanism

temporal development of the current flowing is measured by an oscilloscope.

Currently, experiments with nitrogen dioxide and vaporized mono- and bicyclic nitrated model compounds in a nitrogen flow are performed.

S. Schneider

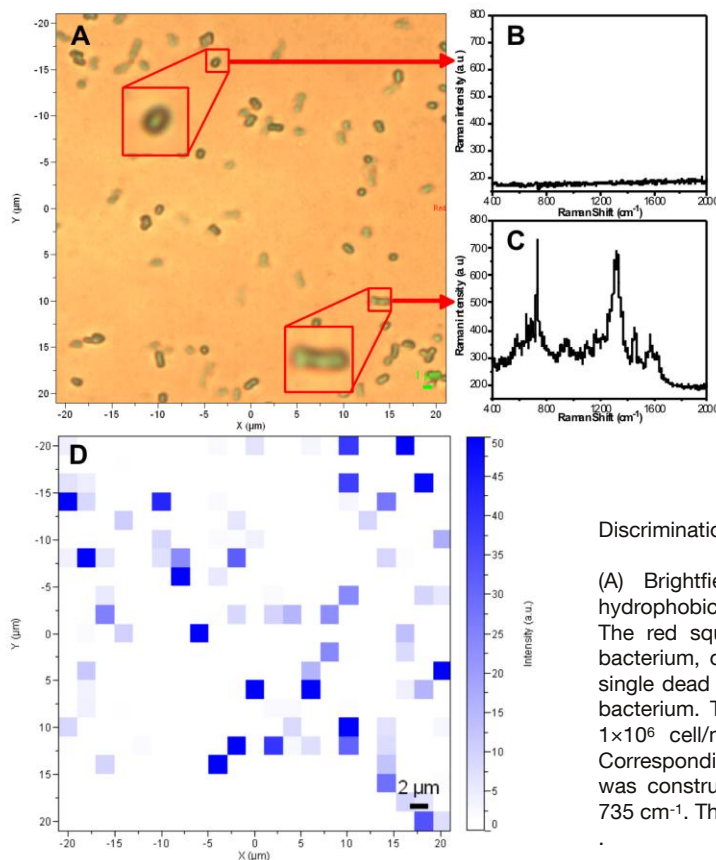
In situ Rapid Counting Live and Dead Bacteria by Label-Free SERS Mapping

Funding: IWC, China Scholarship Council

Cooperation: Max von Pettenkofer-Institut, LMU, Prof. Dr. S. Schubert

Techniques to distinguish between live and dead bacteria in a quantitative manner are in high demand in numerous fields, such as medical care, food safety, public security, as well as basic research. This work demonstrates new nanostructures (Bacteria@AgNPs) and their utility for rapidly counting of live and dead bacteria by SERS. We found that suspensions containing Gram-negative organisms as well as AgNPs give strong SERS signals of live bacteria when generated a certain way. However, no SERS signals is detected from Bacteria@AgNPs

suspensions containing dead bacteria. We successfully demonstrate quantification of different percentages of dead bacteria, both in bulk liquid and on glass surfaces. By using SERS mapping, single cells are detected and counted. Furthermore, different chemicals have been used to elucidate the mechanism involved in this observation. Finally, we used the Bacteria@AgNPs method to detect antibiotic resistance of *E. coli* strains against several compounds used in human medicine. H. Zhou, A. Wieser



Discrimination between single live and dead bacteria.

(A) Brightfield images of 50% dead bacteria on hydrophobic glass slides, the area is 40 μm × 40 μm. The red squares are the original and enlarged single bacterium, objective used 100×. (B) SERS spectrum of single dead bacterium. (C) SERS spectrum of single live bacterium. The total concentration of *E. coli* used was 1×10⁶ cell/mL, a 100× objective was employed. (D) Corresponding SERS image from A. The SERS mapping was constructed on the area of the strongest peak at 735 cm⁻¹. The concentration of *E. coli* is 1×10⁶ cell/mL.

Raman Microspectroscopy Center (Dr. N. P. Ivleva)

Raman Microspectroscopic Analysis of Microplastic Particles in Aquatic Sediments

Funding: DFG (Deutsche Forschungsgemeinschaft)

Cooperation: Prof. Dr. C. Laforsch, University of Bayreuth

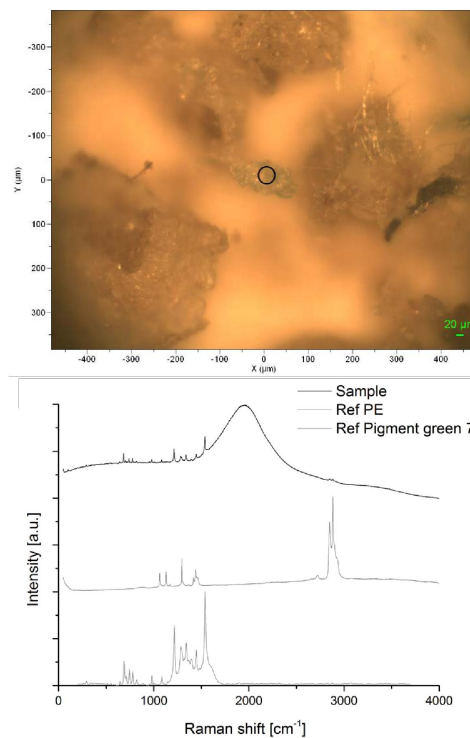
In the last years the risks and concerns about microplastic particles gained awareness as well in the scientific community as in the public media. Microplastic is formed as a result of mechanical, UV- and biological degradation of macroplastic (secondary microplastic) or produced directly for industrial abrasives or care products in cosmetics (primary microplastic). Microplastic is commonly referred to as plastic particles with sizes from 1 μm to 5 mm. However, the discrimination in further size classes is essential for a more specific analysis of the samples. Large Microplastic Particles (L-MPP) is the region from 500 μm – 5 mm, Small Microplastic Particles (S-MPP) is defined as particles from 500 μm – 50 μm and Very Small Microplastic Particles (VS-MPP) includes all particles from 1 μm to 50 μm . But not only the plastic size is a relevant property for the characterization. As plastics are used in numerous application and purposes they are also available in a large scale of color variants. These colorants pose additional harm to the environment because they often contain toxic and hazardous elements.

Contrary to L-MPP and S-MPP, which can also be analyzed by means of IR spectroscopy, Raman microspectroscopy (RM) is the only applicable method for the evaluation of VS-MPP. Raman microspectroscopy is the combination of Raman spectroscopy, which is based on the

inelastic scattering of light, with optical microscopy. With this method a spatial resolution down to 1 μm is possible. RM enables us to not only gain information on the plastic type but also on the used colorants.

We detected microplastic particles without and with colorants in beach sediment samples of the subalpine Lake Garda. We found mainly polystyrene, polyethylene and polypropylene as plastic types. The most prominent colorants were Pigment Blue 15 (Phthalocyanine Blue BN), Pigment Green 7 (Polychloro copper phthalocyanine) and Pigment Red 48 (Permanent Red BBC). Further research will help to develop risk assessment and conservation strategies in order to control environmental pollution with (colored) microplastics.

A. Wiesheu, N. P. Ivleva



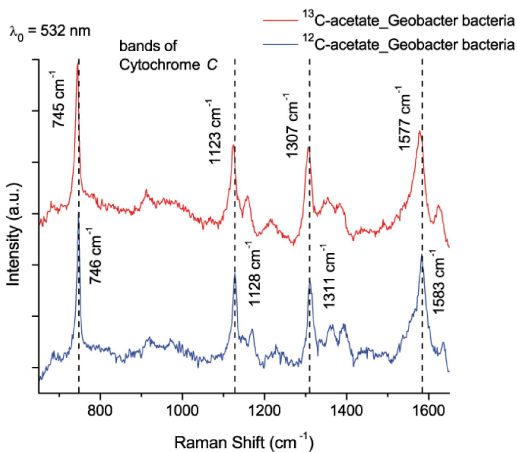
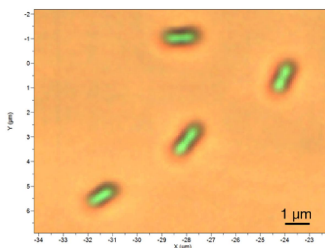
Microscopic image and Raman spectra of a colored small microplastic particle

Stable Isotope Resonance Raman Microspectroscopic Analysis of Groundwater

Funding: Helmholtz Zentrum München (Water Alliance)

Cooperation: Prof. R.U. Meckenstock, PD Dr. T. Lüders, Institute of Groundwater Ecology, Helmholtz Zentrum München

Most microorganisms live in aggregates of cells called biofilms. These multicellular communities (bacteria, protozoa, algae and fungi) are immobilized in a hydrated matrix of biopolymers



Optical microscope image of single *Geobacter* cells; spectra of *Geobacter* cells cultivated with ^{12}C - or ^{13}C -acetate with red shift of the cytochrome c bands

Therefore a rapid and noninvasive analytical method for chemical characterization with high spatial resolution and sensitivity is needed.

Raman microspectroscopy (RM) provides in situ nondestructive chemical characterization of the biofilm matrix in the μm -range without the interference of water.

(extracellular polymeric substances, polysaccharides, proteins, nucleic acids, lipids). Especially water interfaces are a great place for microorganisms to accumulate and form biofilms. They have significant impact in the degradation of water quality-related substances.

However, they are very sensitive to external influences and therefore

Due to the low quantum efficiency of 10^{-6} to 10^{-8} Raman spectroscopy has only a limited sensitivity. This usually leads to long acquisition times, especially in the analysis of single cells with a naturally low biomass. However, an enhancement of the Raman signal is possible with for example resonance Raman microspectroscopy. The resonance Raman effect occurs when the wavelength of the incident laser light coincides with an electronic transition of the molecule. When the microbial sample possesses resonance Raman active substances, such as chlorophyll, cytochrome c or carotenoid a rapid analysis is simply possible by choosing an appropriate laser wavelength. In this project we study the accumulation and degradation of groundwater related substances by means of resonance RM. Stable isotopes (i.e. ^{13}C -labeled compounds) are used to achieve a better understanding of degradation pathways.

For example resonance Raman bands of carotenoid in ^{13}C -labeled microorganisms show a characteristic red shift in their spectrum. The resonance Raman spectra of ^{13}C -labeled *Geobacter* bacteria show a clear red shift of the cytochrome c bands of the bacterial cells. The results should help in understanding the influence of biofilms on the flux, turnover and fate of natural and anthropogenic pollutants in regional water cycles.

P. Kubryk

Raman Analysis of Soil Organic Matter for Improving the Water Holding Capacity

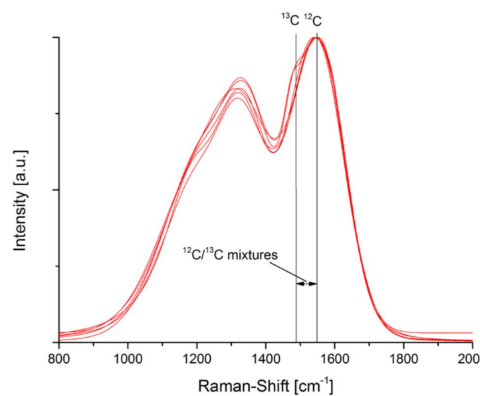
Funding: International Graduate School of Science and Engineering (IGSSE), TUM

Cooperation: Prof. Dr. I. Kögel-Knabner, Chair of Soil Science, TUM

The climate change will lead to alternate rainfall patterns. Less frequent rainfall events with higher intensities are expected. In order to maintain a constant agricultural yield the soil has to store as much rainwater as possible and enable the plants to penetrate and proliferate the soil. In literature a correlation between available water capacity (AWC) and soil organic matter (SOM) is discussed. A higher content in SOM leads through aggregate formation to an increased porosity of the soil. However there is no specific knowledge on the exact mechanisms involved.

The complex and variable structure of the soil leads to high requirements for the analytical method. A suitable technique for the evaluation of soil samples is Raman microspectroscopy (RM), which is based on the inelastic scattering of light. RM enables the non-destructive analysis of soil samples down to a spatial resolution of 1 μm . With the labeling of SOM with ^{13}C -isotopes the fate and transformation in different soil types can be studied. Due to the higher mass of ^{13}C a

specific red shift in the spectra is observed. As the red shift correlates linearly with the amount of ^{13}C , information on the content and distribution in the sample can be gained.



Optical image and Raman spectra of artificial humic acids

Organic amendments in soil will mainly degrade to humic acids, therefore these are studied as a model compound. Artificial humic acid is produced by the reaction of glucose with urea in concentrated chloric acid. Different ratios of ^{13}C to ^{12}C glucose and urea are used and a calibration is established.

For the analysis humic acids surface-enhanced Raman scattering (SERS) is applied. By addition of rough metal surfaces (e.g. Ag or Au) a strong increase of the Raman intensities

can be accomplished. The enhancement can be explained by an electromagnetic effect through surface plasmon resonance and a chemical effect by charge transfer. SERS quenches the fluorescence and enables therefore the analysis of the highly fluorescent humic acid samples.

A. Wiesheu

Bioseparation and Microarray Technology (Dr. M. Seidel)

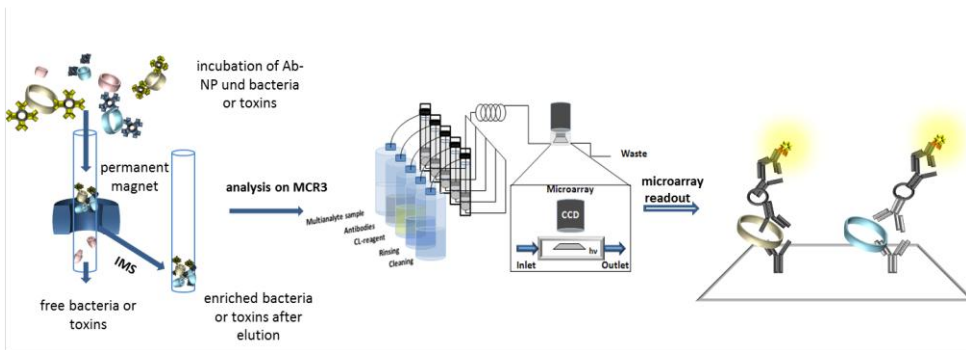
Fast Concentration and Multiplex Microarray Analysis for the Simultaneous Detection of Pathogens and Toxins in Food

Funding: BMBF (Federal Ministry for Education and Research)

Cooperation: Chair of Hygiene and Technology of Milk, LMU Munich; Institute of Veterinary Food Science, JLU Gießen; R-Biopharm AG (Darmstadt)

It is crucial to maintain the food supply chain free of contaminants, as well as hygienically and toxicologically safe. In the case of a contamination, the agent of infection, its origin and all contaminated products have to be immediately identified to minimize risks for the customers.

The rapid enrichment of microorganisms and toxins from liquids (e.g. milk) and solid (e.g. meat, fish) matrices is based on two methods: monolithic immunofiltration (MIF) for liquids and immunomagnetic separation (IMS) for liquids and solids. MIF takes place in monolithic columns with immobilized capture antibodies. In a first experiment with *B. cereus* spores in 100 mL milk, the combination of MIF and antibody microarray analysis on MCR3 achieved better sensitivities. New magnetic nanoparticles that are compatible with food matrices and chemiluminescence readout were investigated.



Combination of immunomagnetic separation (IMS) and sandwich microarray immunoassay on MCR3 for rapid identification of foodborne pathogens

The aim of this project is to develop fast and multiplexed analytical methods to provide a rapid diagnosis and identification of food pathogens and toxins. We use polyclonal and monoclonal antibodies developed by our project partners (LMU and JLU) to establish a rapid screening method for antibodies against pathogenic bacteria based on the microarray analysis platform (MCR3). With *Klebsiella pneumoniae* (alive or inactivated) immobilized on microarray chips, antibodies against these pathogens in sera of rabbits were identified within 20 minutes.

Highly monodisperse oleate magnetic nanoparticles were synthesized and were able to capture *Cronobacter turicensis* in milk with high efficiency. The sensitivity of the sandwich microarray immunoassay on the MCR3 was improved in combination with IMS. These achievements show that current time consuming cultivation techniques might be replaced and food analysis time could be reduced from days to hours. Our methods thus have the potential to provide a fast assessment of the compliance of the product with microbiological criteria laid down for food.

E. Linares, A. Gega, M. Adebar

Concentration and Detection of Waterborne Pathogens for the Inline-Monitoring of Drinking- and Raw Water

Funding: BMBF (Federal Ministry for Education and Research)

Cooperation: Helmholtz-Zentrums für Umweltforschung GmbH; Institut für Mikrosystemtechnik, Universität Freiburg (IMTEK); DVGW-Technologiezentrum Wasser Karlsruhe (TZW); R-Biopharm AG (Darmstadt); GWK Präzisionstechnik GmbH (München); Fraunhofer Anwendungszentrum Systemtechnik (Ilmenau); Berliner Wasserbetriebe (BWB)

The investigation of molecular methods and the construction of a hygiene on-line monitoring (HOLM)-system requires parallel concentration of multiple pathogenic, waterborne bacteria and viruses prior to detection. Using ultrafiltration and a monolith-based adsorption-elution method, a concentrate of a few milliliters is generated from a sample volume of several thousand liters. The macro-concentration is combined with a lab-on-chip-based micro-concentration and nucleic acid extraction module. The extracted nucleic acids are analyzed by a DNA microarray on



In July 2014 the reconstructed ultrafiltration setup was tested under field conditions by the Berlin waterworks in Berlin-Friedrichshagen.

the Munich Chip Reader 3 (MCR3) using isothermal amplification and chemiluminescence detection. In contrast to currently established monitoring systems, the HOLM-system uses the species-specific genome of target pathogens instead of cultivation of bacterial indicators. Besides an enormous time advantage, the HOLM-system is applicable to bacteria and viruses at the same time. Moreover the HOLM-system will contain a module for life-dead discrimination

of target bacteria, thereby revealing the infectious risk for bacterial indicators.

During the first period of the project, the ultrafiltration setup applied for macro-concentration of pathogens (developed in a previous DFG project) was reconstructed and further developed. Prior to field experiments,

the device was tested with tap water samples of 1 m³ spiked with bacteriophage MS2. Approximately 70% of MS2 could be recovered. In July 2014, the setup was brought to Berlin-Friedrichshagen to be tested under field conditions by the Ber-

liner Wasserbetriebe. Experiences obtained during the field experiments will help to further develop the ultrafiltration setup as well as the interfaces between the different modules of the HOLM-system. Besides the ultrafiltration setup, also the device for monolithic affinity filtration is presently reconstructed to achieve a maximum of automation.

A. Kunze, D. Elsäßer

Legionella pneumophila Analysis in Bioaerosols, Water and Human Urine Using a Multiplex Panel of Monoclonal Antibodies on the MCR3

Funding: Bayerisches Landesamt für Gesundheit und Lebensmittelsicherheit, IWC

Cooperation: Bayerisches Landesamt für Gesundheit und Lebensmittelsicherheit; Prof. Lück, TU Dresden

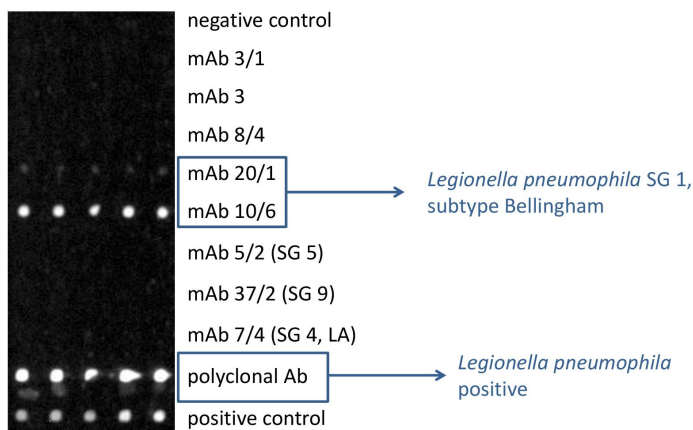
Legionella appear ubiquitous in natural and artificial water sources. People can be infected by inhaling contaminated bioaerosols. Those aerosols can be found in water recoling systems, in showers and

patient (e.g. urine, lung material, etc.)

The standard analysis, done from Legionella reference laboratory in case of infection, takes about 10 days. For the first, quick result, a urine antigene antibody analysis (BINAX®) is done. Afterwards, the grown bacteria were cultivated on selective growth media. However, actual standard analysis methods only allow the detection and identification of *L. pneumophila* serogroup 1, causing more than 80% of all counted legionnaire's diseases, and serogroups 2 - 15 only as sum parameter.

An automated microarray immunoassay (MIA) is a promising serotyping method to rapidly detect all possible serogroups in parallel. A sandwich MIA for Legionella pneumophila serogroup 1 was established on the MCR 3. A panel of high selective and sensitive monoclonal antibodies was multiplexed covalent on the activated surface of the glass chip. The sandwich is performed by using a commercially available, biotinylated polyclonal antibody. Urine of patients infected with legionellosis was tested using ELISA and sandwich chemiluminescence MIA. Bioaerosol samples from factories, using a wastewater treatment plant and surface water from river Isar were equally injected in the multiplex microarray analysis platform MCR 3. The result is very promising for a quick and selective serotyping of *Legionella pneumophila* serogroups in the future.

A. Wunderlich



Multiplex Microarray Chip for *Legionella pneumophila* serotyping – urine sample from infected patient

clarification plants. Regarding the high risk of infection, the detection of *Legionella spp.* has a great impact on the environmental hygiene and medicine. It has to be investigated, in which way the bioaerosol distribution, the origin of the contamination and the infected patients correlate with each other. Bioaerosol samples from factories, breweries, clarification plants and industries which use recoling systems were taken with a cyclone sampler Coriolis µ®. The bioaersols were compared with environmental samples (water, air) and material from the infected

Aerosol Research (Prof. Dr. R. Niessner)

Diffusiophoresis as a New Particle Deposition Mechanism

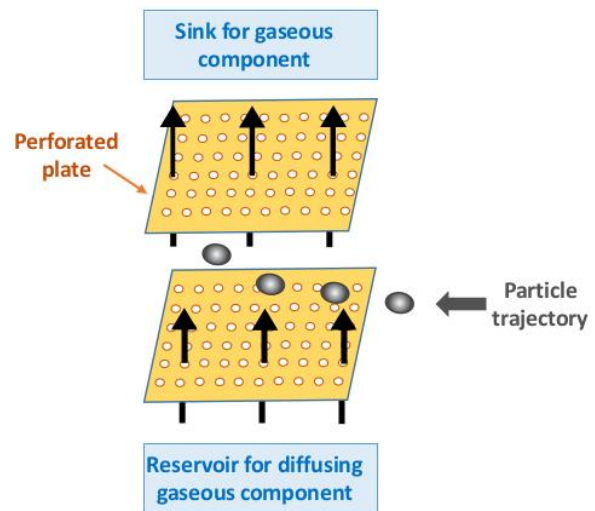
Funding: IWC

Aerosols may contain all kinds of particles like viruses, pollen or diesel soot agglomerates. When inhaling such an aerosol, some of the contained particles are deposited in our respiratory passages. Possible consequences are allergic reactions, asthma or even lung cancer. Amongst others diffusiophoresis is one mechanism that is likely to influence deposition of particles in the lung. Thereby collisions of particles and gaseous components lead to a distraction of the particles from their original trajectories and hence may lead to particle deposition. The directed diffusion of the gaseous components normal to the surface is induced by a concentration gradient. Regarding the lung, such a gaseous component might be oxygen. It diffuses from the inhaled air (high concentration) to the pulmonary surface and is subsequently absorbed (zero concentration). Consequently it is possible that particles move with the oxygen along the concentration gradient towards the surface.

A lot of research has been conducted to be able to estimate how efficient particles are deposited in the different regions of the lung. Thereby the understanding of the details of physical processes leading to particle deposition is necessary. Up to now only little effort was made to experimentally investigate diffusiophoresis. Therefore a diffusiophoretic precipitator was constructed that enables a systematical investigation of this particle deposition mechanism.

The figure shows a schematic of the precipitator. The device consists of a rectangular flow channel with two hole

perforation plates functioning as upper and bottom side of the channel. As shown in the schematic the aerosol (e.g. spark discharge soot particles) flows through the channel. A highly volatile substance (e.g. chloroform) is evaporated from a reservoir, diffuses through the holes and the flow channel in direction to the sink (e.g. activated charcoal). While



Schematic of a diffusiophoretic precipitator

passing the channel particles will collide with the diffusing component, and as a consequence may be deposited at the walls of the flow channel. The fraction of deposited particles is calculated through the ratio of the particle number concentration up- and downstream of the flow channel. Particle number concentrations are determined with the help of a Condensation Particle Counter.

B. Kiwull, B. Dübmann

Reactivity Determination of Soot Originated from Biodiesel Fuels with Temperature-Programmed Oxidation (TPO) and Raman Microspectroscopy (RM)

Funding: FVV (Forschungsvereinigung Verbrennungskraftstoffe), FNR (Fachagentur Nachwachsende Rohstoffe)

Cooperation: Universität Bayreuth (LTTT/BERC), Universität Stuttgart (ICVT), Bergische Universität Wuppertal (Abt. Maschinenbau)

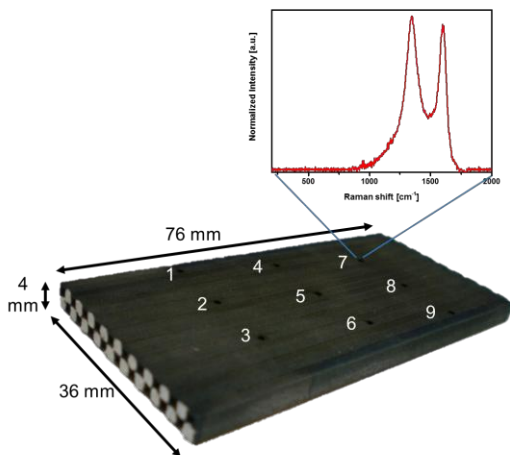
As the sources and amounts of fossil energy carriers are limited, there is a worldwide need to increase the share of energy generated with renewable sources. In Germany, the usage of biofuels is regulated by the

“Biokraftstoffquoten gesetz” (biofuel quota act) which schedules the increase in the blending quota of biofuels up to 8% in 2015.

The task of our institute in this project is, on the one hand, to determine the reactivity of soot, which originates from fuel with increasing fractions of biofuel and is generated under different engine operation conditions, with Temperature-programmed oxidation (TPO) and to link it to the microstructure of the soot, which can be obtained from the Raman microspectroscopic (RM) analysis. Therefore, the soot is oxidized under distinct conditions with a constant temperature ramp. The temperature at which the emission of the gaseous oxidation products, quantified by FTIR, is maximal indicates the soot reactivity. The Raman spectra are taken at different excitation wavelengths in order to correlate the parameters obtained by the method of Multiwavelength Raman Microspectroscopy (MWRM) with the reactivity results.

On the other hand, the change in soot structure during DPF-regeneration is investigated. Therefore, soot in segments of a DPF-structure is analyzed by RM through small holes in the DPF-carrier. The DPFs are analyzed after being loaded with soot as well as after treatment by the project partners from ICVT. There, the soot is heated in inert gas or oxidized at isothermal conditions simulating a short period of an active regeneration step in order to gain information on the processes inside a DPF during regeneration.

M. EB, H. Bladt, N. P. Ivleva



DPF-segment with nine holes and a Raman spectrum of the soot deposited inside the DPF

Burning fuel in the engine of a car or truck generates soot, regardless whether the car is run on biofuel or fossil fuel. In diesel models, the soot is trapped in a diesel particulate filter (DPF) to comply with the emission limits given by law. After a time these filters have to be regenerated, i.e. the soot has to be oxidized to convert the solid matter in gaseous products. Because there is a general lack of information on the physicochemical properties of biofuel-derived soot, the aim of this cooperation project is to gain further insights in the reactivity and microstructure of soot generated with fuels containing different fractions of biodiesel.

Temperature-Programmed Oxidation, Raman Microspectroscopy, and Particle-Conductivity for Diesel Soot Characterization

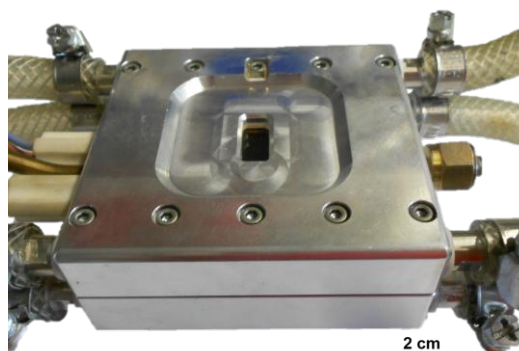
Funding: Audi AG, Ingolstadt

Cooperation: Audi AG, Ingolstadt

Fine and ultra-fine particles originating from natural as well as anthropogenic sources are released in the environment at all time. For example, soot particles are generated in every combustion process in a power plant, a burning fire or a diesel engine. These particles can have a big influence on the environment, the climate or the human health. Therefore, particle emissions are limited and regulated by law. In order to reach these regulations, diesel particulate filters (DPF) are used in diesel cars exhaust to trap the soot. After some time, these filters have to be regenerated, i.e. the soot has to be oxidized to convert the solid matter in gaseous products. It is known that the reactivity of soot, i.e. the temperature at which the soot can be oxidized, is dependent on the soot's microstructure. Hence, effective tools for the determination of the reactivity and microstructure of soot are necessary to allow for a better soot characterization and consequent engine optimization, in order to get reactive soot that can be oxidized faster and at low temperatures.

Therefore a measurement device combining the commonly used most effective soot characterization tools, namely Temperature-Programmed Oxidation (TPO), Raman Microspectroscopy (RM) and electric conductivity in one setup was designed. With TPO, soot is burned at a constant temperature ramp in a defined environment and the gaseous emission products CO and CO₂ are quantified by FTIR to determine the reactivity. Thus, the measurement cell consists of a flow cell, formed by a heatable

steel block (up to 1000°C), on which a sensor with soot can be placed, an insulation and a quartz glass window above and can be connected to a FTIR. With the water cooled aluminum frame, the outside of the cell can be kept at a moderate temperature, which allows one to place it under the Raman microscope. The parameters obtained by RM and conductivity experiments are directly



Integrated measurement cell for TPO, RM, and conductance measurements

related to the soot microstructure. Consequently, the change in the soot microstructure can be monitored /in situ/ by taking Raman spectra through the cell window during heating under distinct conditions.

The next step is to follow the soot burn-off with RM and synchronous monitoring of the emission products with FTIR. By combination of the three individual tools in one setup, comprehensive results will become accessible and a better understanding of the outcomes of the different methods will be achieved.

M. EB, B. Grob, N. P. Ivleva

Particle Number Measurement within Diesel Exhaust

Funding: FVV (Association for Combustion Engine Research, Frankfurt)

Cooperation: Institute of Internal Combustion Engines, Prof. Wachtmeister, TUM

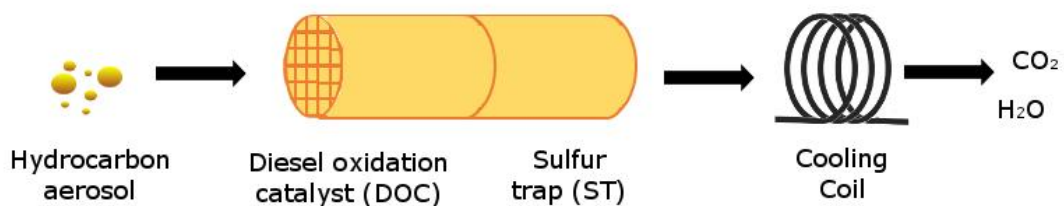
Fine and especially ultrafine particles are considered to be harmful for human health. As diesel-powered vehicles are a significant source for particles in this size range, it is important to limit and consequently reduce the emissions caused by their exhaust. In 2011 a new maximum value, which is based on the number of aerosol particles in exhaust, was established within the European Union. Additionally a new measurement procedure, that includes a pretreatment of the raw exhaust before determination of the particle number, was introduced. The pretreatment involves a separation of volatile and solid exhaust components with a volatile particle remover (VPR) and a quantification of the residual non-volatile particles with a condensation nucleus counter (CNC).

In literature a Catalytic Stripper (CS) is described as one option for the construction of a VPR. This device consists of three parts in a row: diesel oxidation catalyst (DOC), sulfur trap (ST) and cooling coil. Within the DOC volatile particles are evaporated and volatilized hydrocarbons (HC) are catalytically decomposed. The ST consists of a substrate coated with barium and cerium containing compounds. When the exhaust passes through the ST sulfuric acid and sulfur trioxide are irreversibly bound to the surface

and thus removed from the gas phase. In this way the partial pressure of the volatile components is reduced and a recondensation during exhaust cooling is avoided.

To achieve an accurate quantification of solid exhaust particles it has to be assured that volatile components are removed completely from the particle phase. A CS was constructed to evaluate how efficient a CS is able to remove volatile exhaust components. It was shown that the CS is able to remove more than 99 % of H_2SO_4 and HC containing particles in mass concentrations higher than present in diesel exhaust. Additionally, the capacity of the ST was evaluated with H_2SO_4 aerosol (see figure). It became apparent that with the CS it is possible to remove more than 99 % of the H_2SO_4 particles (penetration < 1 %) from the aerosol for more than 20 hours of model aerosol measurement (~ 2 mg H_2SO_4 ; 20 000 h real exhaust loading). Unfortunately, this result is only valid for the home-made CS. Generally, device dimensions and substrate coating (quantity and elemental composition) are varying depending on the manufacturer. With a fixation of CS dimensions as well as substrate coating VPR devices of different manufacturers would be more comparable.

B. Kiwull



Loading of Catalytic Stripper Sulfur Trap with sulfuric acid

Publications

Peer Reviewed Journals

- H. Bladt, N. Ivleva and R. Niessner; Internally Mixed Multicomponent Soot: Impact of Different Salts on Soot Structure and Thermo-Chemical Properties. *J. Aerosol Sci.* 70 (2014) 26-35
- U. Eisold, A. Kupstat, D. Klier, P.-A. Primus, M. Pschenitza R. Niessner, D. Knopp and M. Kumke; Probing the Physicochemical Interactions of 3 – Hydroxybenzo[a]pyrene with Different Monoclonal and Recombinant Antibodies Using Fluorescence Line – Narrowing Spectroscopy. *ABC* 406 (2014) 3387-3394
- B. Grob, J.C. Wolf, B. Kiwull and R. Niessner; Calibration System with an Indirect Photoelectric Charger for Legislated Vehicle Number Emission Measurement Counters in the Single Counting Mode. *J. Aerosol Sci.* 70 (2014) 50-56
- C. Mayrhofer, R. Niessner, and T. Baumann; Hydrochemistry and Hydrogen Sulfide Generating Processes in the Malm Aquifer, Bavarian Molasse Basin, Germany. *Hydrogeology Journal* 22 (2014) 151-162
- N. Mircescu, H. Zhou, N. Leopold, V. Chis, N. Ivleva, R. Niessner, A. Wieser and C. Haisch; Towards a Receptor-free Immobilization and SERS Detection of Urinary Tract Infections Causative Pathogens. *ABC* 406 (2014) 3051-3058
- D. Müller, M. Piller, R. Niessner, M. Scherer and G. Scherer; Metabolomic Investigations in Saliva of Smokers and Non-smokers by a Validated GC-TOF-MS Method. *J. Proteome Res.* 13 (2014) 1602-1613
- D. Müller, C. Degen, G. Scherer, G. Jahreis, R. Niessner and M. Scherer; Metabolomics Using GC-TOF-MS Followed by Subsequent GC-FID and HILIC-MS/MS Analysis Revealed Significantly Altered Fatty Acid and Phospholipid Species Profiles in Plasma of Smokers. *J. Chromatogr. B* 966 (2014) 117-126
- D. Tang, Y. Lin, Q. Zhou, Y. Lin, P. Li, R. Niessner and D. Knopp; Low – Cost and Highly Sensitive Immunosensing Platform for Aflatoxins Using One-step Competitive Displacement Reaction Mode and Portable Glucometer – Based Detection. *Anal. Chem.* 86 (2014) 11451-11458
- X. Wang, R. Niessner and D. Knopp; Magnetic Bead-based Colorimetric Immunoassay for Aflatoxin B1 Using Gold Nanoparticles. *Sensors* 14 (2014) 21535-21548
- S. Lengger, J. Otto, D. Elsässer, O. Schneider, J. Fleischer, A. Tiehm, R. Niessner and M. Seidel; Oligonucleotide Microarray Chip for the Quantification of MS2, PhiX174 and Adenoviruses on the Multiplex Analysis Platform MCR 3. *ABC* 406 (2014) 3323-3334
- R. Niessner; Characterization of Engine - released Soot Nanoparticles – The Many Faces of Soot –. *Angewandte Chemie* 139 (2014) 12366-12379
- C. Palma, K. Diller, R. Berger, A. Welle, J. Björk, J.-L. Cabellos, D. Mowbray, A. Papageorgi, N. Ivleva, S. Matich, E. Margapoti, R. Niessner, B. Menges, J. Reichert, X.-L. Fengi, H. Räder, F. Klappenberger, K. Müllen and J. Barth; Photo – induced C – C Reactions on Insulators Towards Direct Graphitic Patterning. *JACS* 136 (2014) 4651-4658

- M. Pschenitzka, R. Hackenberg, R. Niessner and D. Knopp; Analysis of Benzo[a]pyrene in Vegetable Oils Using Molecularly Imprinted Solid Phase Extraction (MISPE) coupled with Enzyme-Linked Immunosorbent Assay (ELISA). *Sensors* 14 (2014) 9720-9737
- M. Pschenitzka, E.S. Gavrilova, S.A. Tarasov D. Knopp, R. Niessner and O. Epstein; Novel Approach for Quality Control Testing of Release – active Forms of Diclofenac Using Heterogeneous Immunoassay. *Int. Immunopharmacol.* 21 (2014) 225-230
- M. Seidel and R. Niessner; Chemiluminescence Microarrays in Analytical Chemistry. *ABC* 406 (2014) 5589-5612
- A.K. Sharma, M. Saini, S.D. Singh, V. Prakash, A. Das, R.B. Dasan, S. Pande, D.L. Bohara, T.H. Galligan, R.E. Green, D. Knopp and R.J. Cuthbert; Evidence of Toxicity of Diclofenac to a Non-Gyps Vulture and an Aquila Eagle: A Wider Range of Raptor Species May be Threatened by NSAID Misuse. *Bird Conserv. Int.* 24 (2014) 282-286
- E.S. Speranskaya, N.V. Beloglazova, P. Lenain, S. De Saeger, Z. Wang, S. Zhang, Z. Hens, D. Knopp, R. Niessner, D.V. Potapkin and I.Y. Goryacheva; Polymer Coated Fluorescent CdSe-based Quantum Dots for Application in Immunoassay. *Biosensors & Bioelectronics* 53 (2014) 225-231
- A. Szkola, E. Linares, S. Worbs, B. Dorner, R. Dietrich, E. Märtlbauer, R. Niessner and M. Seidel; Rapid and Simultaneous Detection of Ricin, Staphylococcal Enterotoxin B and Saxitoxin by Chemiluminescence Based Microarray Immunoassay. *Analyst* 139 (2014) 5885-5892
- J.-C. Wolf, A. Danner, R. Niessner and C. Haisch; NO₂ Measurement Artifacts in the Presence of Soot. *Anal. Bioanal. Chem.* 406 (2014) 447-453
- H. Zhou, D. Yang, N. Ivleva, N. Mircescu, R. Niessner and C. Haisch; SERS Detection of Bacteria in Water by in situ Coating with Ag Nanoparticles. *Anal. Chem.* 86 (2014) 1525-1533

Books

- R. Bock and R. Nießner; *Trennungsmethoden in der Analytischen Chemie*, deGruyter, Berlin.

Conference Presentations

Oral Presentations

- P. M. Abraham, T. Baumann & G. E. Schaumann, Sorption of untreated and humic acid coated silver nanoparticles to environmental and model surfaces, EGU General Assembly, 27.4.-2.5.2014, Vienna.
- T. Baumann, Pesticide metabolites as tracers in deep groundwater, International Multidisciplinary Conference on Mineral Waters, 8.-11.9.2014, Karlovy Vary, CZ.
- C. Hecht, N. Frank, C. Pletl, T. Baumann & M. Herbrich, Geothermieanlage Sauerlach, Untersuchungen und Maß- nahmen zur Betriebsoptimierung, Der Geothermiekongress, 11.-13.11.2014, Essen.

- N. P. Ivleva, R. Niessner, F.-X. Ouf, Raman Microspectroscopic Analysis of Soot Samples with Different Organic Carbon Content, Conference on Aerosol Technology, 16 - 18 June 2014, Karlsruhe, Germany
- M. Kühn, N. P. Ivleva, R. Niessner & T. Baumann, Stability and effects of natural coatings on engineered inorganic nanoparticles (einp) investigated by surface enhanced Raman spectroscopy (SERS), Internano Conference, 12./13.3.2014, Landau.
- D. Mercier, M. Ben Haddada, M. Hübner, R. Niessner, D. Knopp, C.-M. Pradier, A. Proust, M. Salmain, S. Boujday, Nanostructured Gold Surfaces for Sensitive Biosensors, Biosensors 2014, 27.-30.05.2014, Melbourne, Australia.
- C. Metz, N. P. Ivleva, R. Niessner & T. Baumann, In situ analysis of pore scale processes at biogeochemical interfaces, FH-DGG Tagung, 28.-30.5.2014, Bayreuth.
- S. Oswald, D. Knopp, R. Niessner, First experimental evidence for an enzyme-generated chemiluminescence-induced trans-cis isomerization of chip-immobilized zearalenone in a microfluidic cell of a biosensor, ISBC 2014, 23.-28.06.2014, Uppsala.

Poster Presentations

- T. Baumann, C. Metz & R. Niessner, Colloids at NAPL-interfaces, EGU General Assembly, 27.4.-2.5.2014, Vienna.
- B. Grob, J. C. Wolf, B. Kiwull & R. Niessner, Calibration System with an Indirect Photoelectric Charger for Legislated Vehicle Number Emission Measurement, 28.8.-2.9.2014, Busan (Korea).
- M. Herbrich, C. Hecht, N. Frank, C. Pletl, F. Barenth, R. Niessner & T. Baumann, Scalings in the thermal water system of a geothermal power plant in the Malm aquifer, FH-DGG Tagung, 28.-30.5.2014, Bayreuth.
- M. Hübner, R. Nießner, D. Knopp. Entwicklung einer Mikroarray-basierten immunologischen Bestimmungsmethode für organische Spurenstoffe in der Umwelt, Jahrestagung der Wasserchemischen Gesellschaft, 26.-28.05.2014, Haltern am See.
- M. Hübner, M. Ben Haddada, C. Méthivier, R. Nießner, D. Knopp, S. Boujday, In-depth Analysis of a Self-Assembled PEG Coating on Glass-Type Substrates for Regenerable Immunosensors and Hapten Microarrays, 27.-30.5.2014, Melbourne, Australien.
- N. P. Ivleva, H. K. Imhof, J. Schmid, R. Niessner, C. Laforsch, Contamination of a Subalpine Lake with Microplastic Particles, WASSER 2014, 26 - 28.05.14, Haltern am See (Best Poster Award).
- B. Kiwull & R. Niessner, Investigations on the Removal of Volatile Compounds from Diesel Exhaust Aerosol. Int. Conf. Aerosol Science, 28.8.-2.9.2014, Busan (Korea).
- P. Kubryk, J. Kölschbach, R. Niessner, R. Meckenstock, N. P. Ivleva, Stable Isotope Raman Microspectroscopic Analysis of Groundwater Related Microorganisms and Biofilms, WASSER 2014, 26 - 28.05.14, Haltern am See.
- M. Kühn, N. P. Ivleva, R. Niessner & T. Baumann, Stability and effects of natural coatings on engineered inorganic nanoparticles (EINP) investigated by surface enhanced Raman spectroscopy (SERS), FH-DGG Tagung, 28.-30.5.2014, Bayreuth.

- M. Lafogler, A. Savvatis, F. Wenderoth, A. Seitz-Gutmann, R. Niessner & T. Baumann, Effects of hydrogeochemistry on the long-term hydraulic behaviour of geothermal wells in the Molasse Basin, Bavaria, FH-DGG Tagung, 28.-30.5.2014, Bayreuth.
- C. Metz, N. P. Ivleva, R. Niessner, T. Baumann, Analysis of Pore Scale Processes at Biogeochemical Interfaces in Soil - Quantification of Gradients, Biogeochemical Interfaces in Soil: Towards a Comprehensive and Mechanistic Understanding of Soil Functions, 6.-8.10.2014, Leipzig.
- A.-C. Neumann, C. Haisch, R. Niessner, D. Knopp, Development of a Microbial Fuel Cell for Continuous Monitoring of Small Wastewater Treatment Plants, Jahrestagung der Wasserchemischen Gesellschaft, 26.-28.05.2014, Haltern am See.
- M. Ueckert, U. Steiner, M. Auer, R. Niessner & T. Baumann, High temperature aquifer storage in the Molasse Basin, Bavaria, FH-DGG Tagung, 28.-30.5.2014, Bayreuth.
- M. Ueckert, R. Niessner & T. Baumann, Colloids in the River Inn, EGU General Assembly, 27.4.-2.5.2014, Vienna (Young Student Outstanding Poster Award).
- A. C. Wiesheu, L. Paetsch, C.W. Mueller, I. Kögel-Knabner, R. Niessner, N. P. Ivleva, Raman Microspectroscopy on Stable Isotope Labeled Compounds for Improving the Water Holding Capacity, WASSER 2014, 26 - 28.05.14, Haltern am See.
- A. Wunderlich, C. Lück, R. Niessner, M. Seidel, Rapid and multiplexed detection of Legionella pneumophila serogroups in urine samples by antibody microarrays on the analysis platform MCR 3, Microbiology and Infection 2014, 5.-8.10.2014, Dresden.

Scientific Committees

- T. Baumann, Fate and Transport of Biocolloids and Nanoparticles in Soil and Groundwater, EGU General Assembly, 27.4.-2.5.2014, Vienna (Convener)
- T. Baumann, Internano Conference, 12./13.3.2014, Landau (Scientific Committee)
- T. Baumann, Biogeochemical Interfaces in Soil: Towards a Comprehensive and Mechanistic Understanding of Soil Functions, 6.-8.10.2014, Leipzig (Scientific Board)

Invited Lectures

- T. Baumann, Erschließung unkonventioneller Gasvorkommen durch Fracking, VBEW Vorstandsrat, 21.10.2014, München.
- T. Baumann, Geothermische Nutzung des Malmaquifers im Bayerischen Molassbecken - Von der Balneologie zur Energiespeicherung, TU Berlin, 12.2014, Berlin.
- C. Haisch, SERS on Microorganisms, Inside Raman Seminar 2014, 25.-26. September 2014, Pliezhausen, Germany.
- C. Haisch, Fundamentals and Applications of Photoacoustic Spectroscopy, DAAS Doktorandenseminar, 22.-24. 09.2014, Universität Münster, Germany.
- N. P. Ivleva, Raman Microspectroscopy for Environmental Analysis: Focus on Stable Isotope Technique, 26.11.2014, TUM, Lehrstuhl für Hydrogeologie, Munich, Germany.
- D. Knopp, The Determination of Anti-Polycyclic Aromatic Hydrocarbon Antibodies in Human Blood - a Valuable New Tool for Human Exposure Monitoring?, 7th International Workshop on Agri-Foods Quality and Safety, Oil Crops Research Institute, Chinese Academy of Agricultural Sciences (CAAS), Key Laboratory of Biotoxins, 04.-09.03.2014, Wuhan, China

- D. Knopp, Immunological Methods for Food Analysis With Special Emphasis on Mycotoxin Determination in Grain, 7th International Workshop on Agri-Foods Quality and Safety, Oil Crops Research Institute, Chinese Academy of Agricultural Sciences (CAAS), Key Laboratory of Biotoxins, 04.-09.03.2014, Wuhan, China
- D. Knopp, Bioanalytische Methoden zum Mykotoxinnachweis in Getreide, Bundesanstalt für Materialforschung- und prüfung (BAM), Fachabteilung Analytische Chemie / Referenzmaterialien, 07.07.2014, Berlin.
- D. Knopp, Die analytische Bestimmung von Mycotoxinen und Pharmaka in Lebensmittel- und Umweltproben mit Antikörper-basierten immunologischen Techniken, KNAUER Jubiläums-Seminar „Lebensmittel im Fokus: Wissenschaftliche Sichtweisen in Ämtern, der Industrie und an Universitäten, 21.11.2014, Weihenstephan.
- D. Knopp, The Analytical Determination of Mycotoxins and Pharmaceuticals in Food and Environmental Samples Using Antibody-Based Immunological Techniques, Fuzhou University, 25.11.2014, Fuzhou, China
- D. Knopp, The Analytical Determination of Mycotoxins and Pharmaceuticals in Food and Environmental Samples Using Antibody-Based Immunological Techniques, Suzhou University, 27.11.2014, Suzhou, China
- D. Knopp, Photochemical Isomerization of Zearalenone – a (New) Problem for Immunological Determinations, Oil Crops Research Institute, Chinese Academy of Agricultural Sciences (CAAS), 29.11.2014, Wuhan, China
- R. Niessner, Aktuelle Forschungsergebnisse zur Erfassung und Charakterisierung von Mikroorganismen, VBEW Jahrestagung, 11.3.2014, Coburg.
- R. Niessner, New Tools (Needed) for Monitoring of Water Quality, 17.3.2014, Sorbonne Universities, Paris.
- R. Niessner, Soot Reactivity of Biodiesel, 27.3.2014, FVV Jahrestagung, Magdeburg.
- R. Niessner, Laserlight: Versatile Tool for Chemoanalytical Particle Characterization, 20.5.2014, Universität Freiburg.
- R. Niessner, Combination of Temperature-programmed Oxidation, Raman Microspectroscopy and Particle Conductivity for Diesel Soot Characterization, 26.8.2014, Int. Conf. Aerosol Science, Busan (Korea).
- R. Niessner, Reactivity of Bio Fuel Generated Soot, 27.8.2014, Int. Conf. Aerosol Science, Busan (Korea).
- R. Niessner, Laserlight: Versatile Tools for Chemoanalytical Particle Characterization, 12.11.2014, Leibniz Institut für Analytische Wissenschaften, Dortmund.
- R. Niessner, Mikroarrays & Raman-Spektroskopie zur Detektion von Bakterien und Viren, 1.10.2014, Universität Tübingen.
- M. Seidel, Chemilumineszenz-Mikroarrays für die Kontrolle von Lebensmitteln und Wasser, Institut für Lebensmittelchemie, Universität Hohenheim, 10.7.2014, Hohenheim.
- M. Seidel, Rapid and multiplex analysis of bacteria, viruses, pharmaceuticals or biotoxins by means of chemiluminescence microarrays, Leibniz-Institut für Pflanzengenetik und Kulturpflanzenforschung, 12.6.2014, Gatersleben.
- M. Seidel, Rapid and multiplex analysis of bacteria, viruses, pharmaceuticals or biotoxins by means of chemiluminescence microarrays, Max von Pettenkofer-Institut, 10.6.2014, München.

- M. Seidel, Rapid microarray-based analysis methods for water control - quantification of pharmaceuticals, biotoxins and pathogens, Lehrstuhl für Siedlungswasserwirtschaft der TUM, 5.5.2014, Garching.
- M. Seidel, Bakterien und Viren: Die Herausforderung in der Wasseranalytik, Sitzung des AMA-Wissenschaftsrates, 26.3.2014, München.
- M. Seidel, Multiplexed microarray analysis for the quantification of pharmaceuticals, toxins, and pathogens regarding food and water safety, Bundesamt für Bevölkerungsschutz Labor Spiez, 20.2.2014, Spiez, Schweiz.

Hydrochemical consulting

- Mineralisation control analyses: Bad Abbach, Bad Aibling, Bad Birnbach, Bad Füssing, Bad Griesbach, Bad Gögging, Bad Reichenhall, Bad Rodach, Bad Wörishofen, Bayreuth, Hölle, Kondrau, Treuchtlingen, Lipik (Croatia), Memmingen, Neumarkt i. d. Opf., Sibyllenbad, Straubing, Utting, Weißenstadt
- Hydrogeological and hydrochemical expertises (mineral water, spa water): Bad Gögging, Bad Griesbach, Bad Wimpfen, Garching
- Deep Hydrogeothermal Energy Exploration: Aschheim, Pullach, Sauerlach, Waldkraiburg, Pullach, Sauerlach

Theses

PhD Theses

- Dipl.-Chem. Henrike Bladt: Oxidationsreaktivität von Rußen: Einfluss intern gemischter Mineralien sowie Kraftstoff- und Abgaszusammensetzung
- MSc Chem. Simon Donhauser: Entwicklung und Validierung eines automatisierten DNA-Mikroarrays zur Detektion von humanpathogenen Bakterien in Trinkwasser
- Dipl.-Ing. FH Daniel Müller: Metabolomics Investigations in Body Fluids of Smokers and Non-smokers
- Lehramt Biol. Chem. Daniela Rascher: Entwicklung, Charakterisierung und Anwendung eines optischen Immunosensors zur Bestimmung von Procalcitonin in humanem Plasma und Vollblut
- MSc Chem. Agathe Szkola: Sensitiver und paralleler Nachweis von Biotoxinen mittels Chemilumineszenz – Durchfluss – Mikroarrays
- MSc Chem. Klaus Wutz: Entwicklung eines Immuno-chips zur simultanen Detektion von Antikörpern gegen zoonotische Pathogene in Schweineseren
- MSc Chem. Haibo Zhou: Label-Free Applications of SERS for Bacteria Analysis

M.Sc. Theses

- BSc Chem. Björn Düßmann: Diffusiophorese unter laminaren Bedingungen – Theoretische und praktische Untersuchungen

Cand. Staatsexamen Leb. Chem. Carolin Hartmann: Development and Application of a BOD-Sensor Based on a Microbial Fuel Cell

BSc Chem. Joachim Nagler: Method Development for Determination of Monoamines in Mice Brain and Investigation of Neurotransmitter Networks in Wildtype and Knockout Mice

BSc Chem. Aleksandra Stanojlovic-Collin: Synthese und Charakterisierung magnetischer Nanopartikel und deren Anwendung in der immunomagnetischen Separation

B.Sc. Theses

Philipp Anger: Raman-analyses of Microplastic Particles in Limnic Ecosystems

Jan Berger: Immunologischer Nachweis von Diclofenac mit monoklonalen Antikörpern in Trinkwasser

Jessica Beyerl: Bestimmung der Matrixeinflüsse von zwei monoklonalen Antikörpern gegen Cyanotoxine hinsichtlich ihrer Anwendung für die affinitätschromatographische Abreicherung von Microcystin-LR aus Wasserproben

Thomas Hinkofer: Bestimmung der Transporteigenschaften von Fluoreszenzfarbstoffen für den Einsatz in der tiefen Geothermie mit Säulenversuchen

Marianne Volkmar: Bestimmung der gebundenen Microcystin-LR Menge an unterschiedliche Immunoaffinitäts-Supports mittels indirekt kompetitiven ELISA

Institute Colloquia

Dr. Martin Obst, Universität Tübingen, Center for Applied Geoscience, Environmental Analytical Microscopy: How Analytical Light, X-ray and Electron Microscopy Help to Further our Understanding of the Fate of Contaminants in the Environment (8.1.2014)

PD Dr. Wolfgang Fritzsche, Institut für Photonische Technologien Jena, Department Nanobiophotonik: Bioanalytics Using Single Plasmonic Nanostructures (20.1.2014)

PD Dr. Rudolf Jörres, Institut und Poliklinik für Arbeits-, Sozial- und Umweltmedizin, Klinikum Universität München: Volatile Compounds in Exhaled Air as Potential Markers of Disease - Clinical Perspectives and Challenges (4.2.2014)

Prof. Dr. Gerald Urban, Institut für Mikrosystemtechnik – IMTEK, Universität Freiburg: Micro- and Nanosystems for Bioanalytical Devices (10.2.2014)

Prof. Dr. Thilo Hofmann, Department of Environmental Geosciences, Universität Wien: Hydrogeology & Nanoparticles – Challenges and Trends (13.2.2014)

Prof. Dr.-Ing. Ralf Moos, University of Bayreuth, Chair of Functional Materials: Sensors for Automotive Emission Control: (19.2.2014)

Prof. Dr. Aymelt Itzen, TU München, Fachgebiet Proteinchemie: Posttranslational Protein Modifications of Small GTPases During Legionella Infections (28.2.14)

PD Dr. Martin Elsner, Helmholtz Zentrum München, Institute of Groundwater Ecology: Reaktive Tracer in molekularen Strukturen: Isotopenanalytik von Spurenschadstoffen zur Aufklärung von Abbauprozessen im Wasserkreislauf (10.3.2014)

- Prof. Dr. med. Sören Schubert, Max von Pettenkofer-Institut, Lehrstuhl für Bakteriologie, LMU München: MALDI-TOF MS as a Diagnostic Tool in Clinical Microbiology - Opportunities and Limitations (15.4.2014)
- Dr. Kannan Balasubramanian, Max-Planck-Institute for Solid State Research, Stuttgart: Label-Free Electrical Biodetection Using Carbon Nanostructures (13.5.2014)
- Priv.-Doz. Dr. Udo Conrad, Leibniz-Institut für Pflanzengenetik und Kulturpflanzenforschung (IPK-Gatersleben): Nanobodies-isolation, Plant Based Expression, Purification and Functional Characterization in Vitro and in Vivo (19.5.2014)
- Prof. Dr. Bernhard Lendl, Vienna University of Technology, Institute of Chemical Technologies and Analytics: Mid-IR Quantum Cascade Lasers: A Promising Light Source for Use in Analytical Chemistry (5.6.2014)
- Prof. Dr. Bernadett Weinzierl, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institute für Physik der Atmosphäre: Long-range Transport of Mineral Dust and Black Carbon – Results from Measurements with the DLR Falcon Research Aircraft (3.7.2014)
- Prof. Dr. Guenter Gauglitz, Institute for Physical and Theoretical Chemistry, Universität Tübingen: Optical Sensors for Diagnostics and Environment (8.9.2014)
- Prof. Dr. Thomas Brück, TU München, Fakultät für Chemie, Fachgebiet Industrielle Biokatalyse: Sustainable Bioprocess Development: New Process Options for Specialty Chemicals and Biofuel in the 21. Century (17.11.2014)
- Prof. Dr. Andreas Schaeffer, University RWTH Aachen, Institute for Environmental Research: Long Term Fate of Chemicals in Soil (2.12.2014)
- Dr. Gilbert Nöll, Universität Siegen, Dept. Chemie-Biologie, Organische Chemie: Investigation of DNA and Protein-Modified Surfaces by SPR, SPFS, QCM-D and Electrochemistry (16.12.2014)

External Tasks and Memberships

T. Baumann

Bayer. Fachausschuss für Kurorte, Erholungsorte & Heilbrunnen	Deputy Member
VBEW Arbeitskreis Wasserschutzgebiete	Guest Member
Arbeitskreis Spurenstoffe im Umweltcluster Bayern	Member
Science of the Total Environment	Guest Editor
Journal of Contaminant Hydrology	Guest Editor

C. Haisch

Kommission Reinhaltung der Luft im VDI und DIN - Normenausschuss: Unterausschuss Messen von Partikeln in der Außenluft - Bestimmung der Partikelanzahl	Member
--	--------

D. Knopp

Chromatographia	Editorial Advisory Board
Ecotoxicology and Environmental Safety	Editorial Advisory Board
International Journal of Environmental Research and Public Health	Editorial Advisory Board

School of Chemical Engineering, National Technical University of Athens (NTUA), Greece. Election committee	Member
--	--------

R. Nießner

Bayer. Fachausschuss für Kurorte, Erholungsorte & Heilbrunnen	Member
Heinrich-Emanuel-Merck Award	Jury Head
Hong Kong University Grants Committee, Theme-based Research Scheme, Selection Committee	Member
fms_ProcesNet-Gemeinschaftsausschuss Sensoren und Sensorsysteme (DECHEMA)	Member

Analytical Chemistry	Associated Editor
Analytical & Bioanalytical Chemistry	Advisory Board Member
Analytical Sciences	Advisory Board Member
Annual Review of Analytical Chemistry	Editorial Committee Member
Fresenius' Environmental Bulletin	Advisory Board Member
International Journal of Environmental Analytical Chemistry	Advisory Board Member
Microchimica Acta	Advisory Board Member
Talanta	Advisory Board Member
Toxicological & Environmental Chemistry	Advisory Board Member

M. Seidel

Kommission Reinhaltung der Luft im VDI und DIN - Normenausschuss: Unterausschuss Messen und Bewerten von Legionellen	Member
Kommission Reinhaltung der Luft im VDI und DIN - Normenausschuss: Arbeitsgruppe "Bioaerosole und biologische Agenzien – Luftgetragene Mikroorganismen und Viren"	Member
Spiegelgremium zur CEN/TC 264/WG 28 „Microorganisms in ambient air"	Member
Temporärer Arbeitskreis bei DECHEMA „Biosicherheit und biologisches Monitoring“	Head
Fachgruppe für „Viren und Parasiten“ bei der Wasserchemischen Gesellschaft in der GDCh	Member

Teaching

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

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

Graduate Course in Analytical Chemistry: Lecture in Organic Trace Analysis-Physical and Chemical Separation Methods (Nebenfach Analytische Chemie: Vorlesung Organische Spurenanalytik-Physikalisch-chemische Trennmethoden); Niessner

Graduate Course in Analytical Chemistry: Lecture in Organic Trace Analysis-Applications of Selective Receptors (Nebenfach Analytische Chemie: Vorlesung Organische Spurenanalytik-Nutzung selektiver Rezeptoren); Niessner, Seidel

Graduate Course in Analytical Chemistry: Lab in Organic Trace Analysis (Nebenfach Analytische Chemie: Kurspraktikum Organische Spurenanalytik); Niessner, Seidel

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

Trace Analysis Techniques (Spurenanalytische Techniken); Niessner, Knopp, Haisch

Industrial Chemistry (M.Sc.) GIST TUM-Asia

Lecture in Bioengineering & Bioprocessing; Seidel

Hydrochemistry; Niessner

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

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

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

Applied Hydrogeology (Angewandte Hydrogeologie); Baumann

Contaminant Hydrogeology (Transport von Schadstoffen im Grundwasser); Baumann

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

Technical Hydrogeology (Technische Hydrogeologie); Baumann

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

Hydrogeochemical Modelling (Hydrogeologische Modellierung II); Baumann

Hydrogeological Field Lab (Hydrogeologische Feldmethoden); Baumann

Hydrogeological Mapping (Hydrogeologische Kartierung); Baumann

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

Water Chemistry I (Wasserchemie I); Niessner

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

Hydrochemical Lab (Hydrochemisches Praktikum); Knopp, Baumann

Biosciences (B.Sc./M.Sc.)

Analytical Chemistry - Separation
Techniques, Chemical and Biochemical
Sensors (Analytische Chemie -
Trenntechniken, chemische und
biochemische Sensoren); Knopp

Biochemical and Molecular Biological
Methods in Environmental Analysis I -
Immunological methods; Sensor
techniques (Biochemische und
molekularbiologische Verfahren in der
Umweltanalytik I - Immunologische
Methoden, Sensor Techniken); Knopp

Biochemical and Molecular Biological
Methods in Environmental Analysis II -
Enzymatic methods; DNA Probes
(Biochemische und molekularbiologische
Verfahren in der Umweltanalytik II -
Enzymatische Methoden, DNA-Sonden);
Knopp

Equipment

Hydrogeology

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

Großhadern Unsaturated Zone field laboratory (10 m deep)

1 Analytical Autoclave, Büchi Midiclave for sorption experiments

Dioxin Laboratory

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

Aerosol Research

1 Aerosol chamber (1 m³)

1 Aerosol flow tube (10 L)

1 Ozone analyzer (UV absorption)

1 NO/NO₂ analyser (Chemiluminescence)

2 Aerodynamic particle sizers (0.5-25 µm)

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

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

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

1 High-Volume filter sampler (PM 2.5)

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

2 Diffusion batteries (5-300 nm)

5 Condensation nucleus counters

3 Electrostatic classifiers (10-1000 nm)

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

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

1 Floating bed aerosol generator (powder dispersion)

1 Rotating brush aerosol generator (powder dispersion)

1 Tube furnace

1 Cyclone Impinger (Coriolis µ, Berlin)

1 Micro soot sensor with dilution unit

Bioseparation

1 Crossflow-ultrafiltration unit (6 m²-hollow fibre module, Inge-AG)

1 Munich Microorganism Concentrator (MMC 3)

1 Monolithic Affinity Filtration Unit

Molecular Biology

1 Biacore X100, General Electric

1 Real-time PCR (Light Cycler 480, Roche)

Microarray Technology

2 Chemiluminescence Microarray Reader (Immunomat, IWC)

4 Chemiluminescence Microarray Reader (MCR 3, GWK GmbH)

1 Ink-Jet Microdispenser (SciFlexarrayer 31, scienion)

2 Contact Microarrayer (BioOdyssee Caligrapher, BioRad)

Microbiology

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

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

3 Clean benches

1 Microbiological Incubator (BD 53, Binder)

1 Autoclave (Century 2100, Prestige Medical)

1 Autoclave (SHP Steriltechnik)

Standard Lab Equipment

1 Lyophilizer (Alpha 1-4 LSC, Christ)

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

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

1 Refrigerated Centrifuge (Universal 320R, Hettich)

1 Climatic chamber (Mettmert HCP 108)

2 Fluorescence reader systems, time-resolving

3 Photometric reader systems

1 384-channel washer, Biotek

1 Turbidometer (WTW GmbH)

1 Nanophotometer (Implen GmbH)

Chromatography and Particle Separation

- 3 GCs with FID, NPD, ECD, TEA, and AED
- 1 Orbitrap-based benchtop MS, Exactive/HCD-System, Thermo Fischer
- 1 GC/MS, VG Autospec
- 1 GC/MS, Shimadzu
- 1 Portable Micro-GC, MITEC
- 1 Asymmetrical Field-flow-fractionation system, Postnova
- 2 Concentrators for dynamic headspace analysis
- 4 HPLC, UV/VIS array detector, programmable fluorescence detector
- 1 Capillary electrophoresis system
- 1 Ion chromatograph, Dionex 4500 i
- 1 Ion chromatograph, Dionex BioLC (Photodiode Array Detector, Electrochemical Detector)
- 1 Ion chromatograph, Metrohm 881
- 1 LC system, ECONO
- 1 Preparative HPLC
- 1 Zetaphometer, SEPHY

Elemental Analysis

- 1 TXRF, Atomika EXTRA II a
- 1 Flame-Photometer, Eppendorf ELEX 6361
- 2 AAS systems with flame atomization, electrothermal atomization, hydrid system, Perkin-Elmer PE 3300, ELAN 4100
- 1 ICP-MS, Perkin-Elmer ELAN 6100

Laser

- 2 He/Ne-laser
- 5 Nd-YAG-laser, pulsed
- 1 Nd-YAG Laser 2 W cw, 532 nm narrow band
- 3 Nd-YAG-laser, cw
- 1 CO₂-laser
- 3 Dye-laser (tunable with frequency doubler)
- 5 N₂-laser
- 8 Diode-lasers (600-1670 nm; up to 2 W CW)
- 1 Laserdiode array with 10 diodes (0.8 µm - 1.8 µm)
- 1 Laserdiode with external resonator
- 2 Optical parameter oscillator (410 nm - 2.1 µm)

Optoelectronics/Spectrometer

- 1 Rowland spectrometer
- 2 Echelle spectrometer
- 1 ICCD spectrometer system
- 1 FTIR-Spectrometer, Thermo Scientific Nicolet 6700
- 1 Fluorescence spectrometer, Perkin Elmer LS-50
- 1 Fluorescence spectrometer, Shimadzu RF 540
- 1 Fluorescence spectrometer, Shimadzu RF 5301 PC
- 1 UV/VIS spectrometer, Beckman DU 650
- 1 UV/VIS spectrometer, analytic jena Specord 250 plus
- 1 UV/VIS spectrometer, analytik jena Spekol 1500
- 2 Boxcar integrator
- 4 Digital storage oscilloscopes (400 MHz, 500 MHz)
- 3 Optical multichannel analysators with monochromators, time-resolving
- 1 Wavemeter

SEM/Microscopy

- 1 SEM/EDX system
- 1 Polarisation microscope for phase analysis
- 1 Fluorescence microscope
- 1 Image analysis software for automated image processing
- 1 Inert gas glovebox
- 1 Laminar flow box

Raman-Microscopy

- 1 Laser Raman microscope, Renishaw 2000 (514/633/785 nm)
- 1 Laser Raman microscope, Horiba LabRam HR (532/633/785 nm)
- 1 Temperature controlled stage (-196°C - 600°C, Linkam THMS 600)

Sum Parameters

- 2 Coulostat for C quantification, Coulomat 702
- 1 DOC analysator, UNOR 6 N
- 1 TOC analysator, TOCOR 2
- 1 AOX/TOX, Sigma

Staff 2014

Staff

Univ.-Prof. Dr. Reinhard Niessner
PD Dr. Thomas Baumann
PD Dr. Christoph Haisch
Dr. Natalia P. Ivleva
Dr. Elisangela Linares (-11/14)
Prof. Dr. Dietmar Knopp
PD Dr. Michael Seidel

Birgit Apel
Christine Beese
Roland Hoppe
Joachim Langer
Susanne Mahler
Cornelia Popp
Christine Sternkopf
Christa Stopp
Sebastian Wiesemann

Mira Kolar
Hatice Poyraz

PhD Students

MSc Pharm. Biol. Manuela Adebar (11/14-)
Dipl.-Phys. Christoph Berger
Dipl.-Chem. Henrike Bladt (-10/14)
MSc Chem. Simon Donhauser (-7/14)
Dipl.-Biol.-Ing. Dennis Elsäßer
MSc Chem. Michaela Eß
Dipl.-Phys. Benedikt Grob (-2/14)
Dipl.-Ing. Moritz Herbrich (-6/14)
MSc Chem. Maria Hübner
MSc Chem. Bettina Kiwull
MSc Chem. Patrick Kubryk
MSc Geol. Melanie Kühn
MSc Chem. Andreas Kunze
MSc Ing. Hydrogeol. Mark Lafogler
MSc Chem. Verena Meyer
MSc Chem. Anna-Cathrine Neumann
MSc Chem. Michael Pschenitzka (-3/14)
Dipl.-Chem. Kathrin Schwarzmeier (-7/14)
MSc Chem. Klemens Thaler
MSc Geol. Martina Ueckert
MSc Chem. Xu Wang
MSc Chem. Alexandra Wiesheu
Leb. Chem. Anika Wunderlich
MSc Chem. Haibo Zhou

External PhD Students

MSc Chem. Michael Göttel (10/14-)
Dipl.-Biol. Carmen Kocot (-5/14)
Dipl.-Ing. Daniel Müller (-6/14)
MSc Biol. Johannes Otto
Staatsexamen Lehramt Daniela Rascher (-6/14)
Dipl.-Biol. Michael Schmalenberg

Diploma Students / Master Students

BSc Chem. Björn Düßmann (1/14-7/14)
Cand. MSc Chem. Alda Gega (4/14-10/14)
Cand. Staatsexamen Leb. Chem. Carolin
Hartmann (4/14-9/14)
Cand. MSc Leb. Chem. Maryam Sandhu (10/14-)
BSc Chem. Stefan Schneider (9/14-)
BSc Chem. Aleksandra Stanojlovic-Collin (-7/14)
BSc Chem. Carmen Torggler (10/14-)

External Master Students

BSc Chem. Joachim Nagler (5/14-10/14)
BSc Ind. Chem. Maxine Tam (9/14-)
BSc Chem.-Ing. Sebastian Weiker (8/14-)

Bachelor Students

Yunus Aynur (11/14-)
Jan Berger (4/14-6/14)
Jessica Beyerl (8/14-10/14)
Thomas Hinkofer (3/14-5/14)
Lukas Kutschera (11/14-)
Marianne Volkmar (5/14-7/14)

Guests and Research Fellows

Prof. Dr. Elena Kireeva, Moscow State University
(10/14-12/14)

Student Assistants

Philipp Anger (3/14-10/14)
Jan Berger (10/14-12/14)
Florian Furlinger (9/14-12/14)
Luis Klinksik (9/14-11/14)
BSc Chem. Selina Muffler (8/14-9/14)
BSc E I Elisabeth Preuß (9/14-12/14)
BSc Geol. Matthias Staudacher (10/14-)
BSc Geol. Maximilian Walter (9/14-)
BSc Chem. Carina Wismeth (11/14-)