Technische Universität München

Annual Report 2011

Institute of Hydrochemistry and Chemical Balneology
Chair for Analytical Chemistry

The institute and the director turned 60 last year, congratulations

Institute of Hydrochemistry and Chemical Balneology
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Editor: Dr. Thomas Baumann

Editorial

Dear coworkers, friends, and colleagues,

we are looking back at a year in which the concept of the hydrologic cycle had been brought to the attention of officials at the federal and state government level. The hydrologic cycle seems to be trivial to the scientific community, however, only few processes controlling the fate of contaminants in water, soil, and air have been understood completely. DFG priority programs and research groups and initiatives of the Helmholtz-Centre emphasize the role of interfaces as key to quantify long-term behaviour of contaminants.

This type of research requires sensitive and fast analytical techniques with high spatial and temporal resolution. For instance, gold nanoparticles were used as a analytical tool creating a nucleus for enhanced photoacoustic effects and serve as a core to link to bioanalytical receptors. Using Raman microspectroscopy, the first label-free online analysis of microorganisms captured by antibodies on a chip has been developed.

As environmental standards are raised, our old experience in the characterization of the chemical reactivity is requested again. In a cooperation with Moscow State University we are leading the research around soot from combustion to a new dimension. Internally mixed carbon aerosols show an increased reactivity under thermal oxidative treatment. This seems to be one route for effective exhaust treatment, desperately sought for by car manufacturers.

Coming to the hardware developed at the institute: the automated chip reader platform, MCR3, is now completely commercialised. A thorough validation period since early 2011 was successfully completed these days. Several food monitoring institutions now run field tests in production environments and we expect the official launch by the end of this year.

Different matrix, same story: the newly developed two-channel photoacoustic diesel exhaust sensor (online analysis of NO_2 and soot aerosol in parallel) has reached the level of transfer to the application. First tests under real-world conditions were very promising. Due to the EURO 6 guideline for exhaust depletion, there is a great need for such sensor system.

The world became a little less comfortable for viruses in drinking water: thanks to the enrichment procedures developed at the institute, viruses now can now be detected, at least. We consider this a major step to effective water hygiene control, especially in a time where waterworks are usually not able to monitor viruses at all, as there is no other tool to enrich some 32 m^3 of water to a 1 mL sample, which then can be processed by PCR or ELISA analysis.

As expected, the teaching load increased badly. The number of first-year students almost doubled, with two years of A-level pupils rushing to the university in parallel due the transition to a 8-year secondary school. Thanks to the Bologna system we spend more time preparing and correcting written exams than in personal conversation. While admission to TUM is easier and students coming from all over the world, the quality has to be maintained, hence thorough selection is a must.

The future of the institute may become exciting. First ideas were born to aggregate several institutes and professorships to a “TUM Centre for Water Research”. While we continue working hard to bring this idea to life, it's still a vision.

Finally, I'd like to thank all of you, coworkers, friends, and colleagues for your continuous support and for making this past year an enjoyable experience

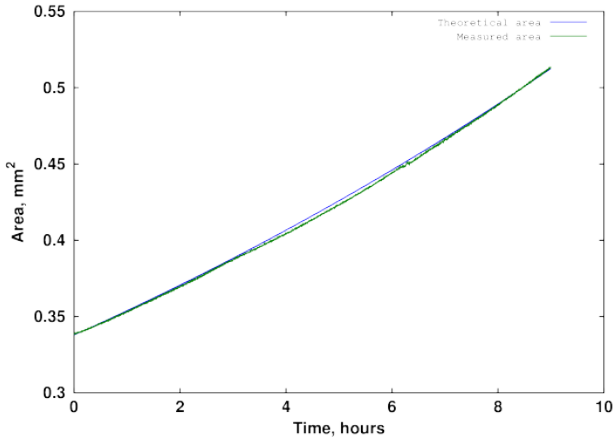
Reinhard Niessner

Hydrogeology (PD Dr. T. Baumann)

Investigating Biogeochemical Interfaces in Soil Using Sensor Micromodels and Raman Microscopy

Funding: DFG
Cooperation: Partners in the DFG Priority Programme SPP 1315

The biosphere controls the fate and the degradation of pollutants, thus the effects of chemicals on the growth and behavior of bacteria need to be understood. The pore scale processes in the biosphere require adequate tools for visualization and quantification. For example, batch experiments, fail at reproducing limited spatial access to interfaces which effect reaction rates. Therefore we apply micromodels, pore structures etched into silicon wafers, to assess the complex interplay between living the organisms and the organic as well as the inorganic matrix material in a porous system.



Growth rate of a gas bubble produced by P. *denitrificans* in the micromodel

Using micromodels and *Paraccocus denitrificans* as a model organism we observed the formation and activity of a biofilm from the very beginning. At first one half of a micromodel was inoculated with a suspension of *P. denitrificans* in diluted culture medium, while through the other half isotonic and sterile saltwater was pumped. After this incubation step, the bacterial suspension was changed to a nutrient feed solution

After 10 days of cultivation we observed the development of gas bubbles in the micromodel pore network. The growth of one gas bubble was recorded over a time period of 9 hours and evaluated using automated image processing. The Figure shows the area of the gas bubble over time, which is proportional to its volume. For the evaluation we assume that there is a monolayer of bacteria at the bottom of the micromodel and that only the bacteria under the bubble contribute to the growth of the bubble. We also assume that the bacteria are using an anaerobic pathway to produce nitrogen. The water used was saturated with nitrogen and oxygen. Therefore we also have to consider partitioning of oxygen from the solution into the gas bubble according to the partial pressures and depending on the gas-water interface area and the flow conditions.

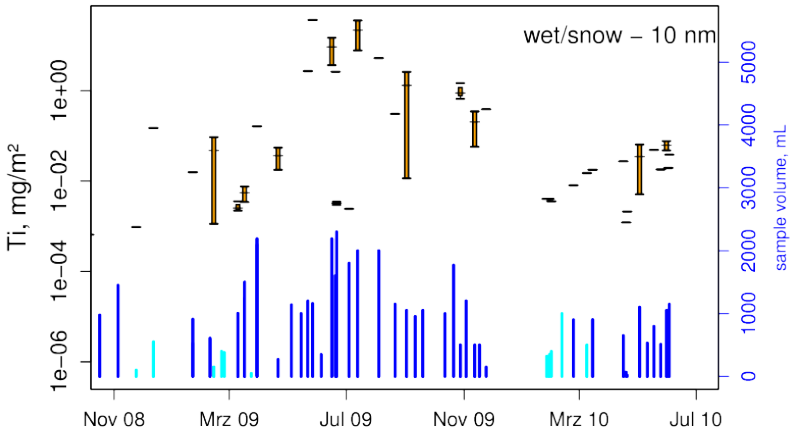
We also assume an increased bioavailability of nutrients for the bacteria in this experiment. Due to the surface tension a gas bubble may swap its position if its size exceeds a certain value, depending on the local topology. This alternation of the residual place may result in an alteration of the flow pathways, which occurred at several spots in the micromodel as long as the gas production was in progress.

C. Metz

Nanoparticles in the Unsaturated Zone

Funding: Gottlieb Daimler and Carl Benz-Foundation

In the light of increasing use of engineered nanoparticles and reports of reports of adverse effects of nanoparticles on aquatic ecosystems and possible health issues, assessment of the transport of nanoparticles is of high importance. In this study we address the transport of airborne nanoparticles through the unsaturated zone in an urban environment.



Deposition of TiO_2-nanoparticles and precipitation (blue) at the Großhadern site

Aquifers and soils are the primary filter systems to remove engineered nanoparticles. These effects are used, e.g., for bank filtration. Recent flooding events, on the other hand, show the limited capacity of this filter. While engineered nanoparticles are tailored to specific applications, one has to assume that they nonetheless interact with dissolved organic matter (DOM) present in surface water and top soil in larger quantities. A coating with DOM has a stabilizing effect on most nanoparticles. Thus, a transport of engineered nanoparticles through the soil seems likely.

A monitoring program was performed at the Munich vadose zone field laboratory, a shaft reaching from the top soil to the groundwater table at 10 m below the ground surface. Wet and dry deposition were collected and analyzed to assess the input function. Seepage water was collected and analyzed in nine depths to assess the transport of nanoparticles (see Fig.). For all samples the size distribution and the elemental composition of the particles was measured using ultrafiltration, AF^4 and ICP/MS.

Nanoparticles deposited during dry periods may accumulate on the plant leaves and on the top soil. Here a first interaction with organic matter occurs. Heavy rainfall after a dry period will mobilize the nanoparticles. Through cracks in the top soil, preferential flow can transport the surface modified particles to the groundwater. During winter, particles are deposited on the snow cover. Sublimation of snow may lead to relatively high concentrations in the remaining snow. Cracks in the top soil caused by freezing ease the transport of nanoparticles together with the melting snow. During winter, however, aging and masking of the nanoparticles should be different.

Laboratory experiments in undisturbed soil columns indicate that the transport of unaltered, dispersed nanoparticles (TiO_2, SiO_2) is very limited. Filtration efficiency is on the order of 98.5% for a sand column which was 10 cm long. This is in contradiction to field observations and underlines the importance of preferential flow and masking for nanoparticle transport.

S. Huckele

Hydrochemistry of the Malm Aquifer

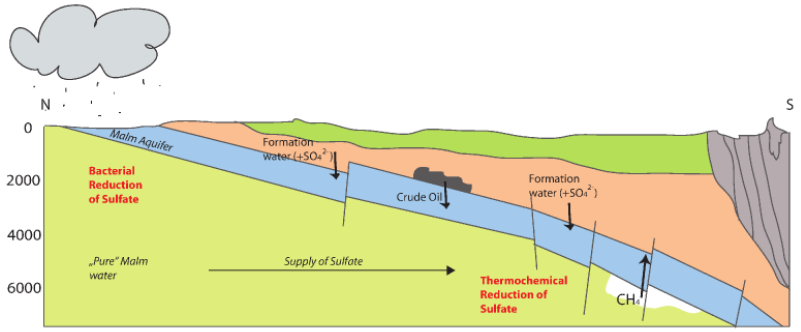
Funding: BMU
Cooperation: Prof. Schneider (FU Berlin); Erdwerk GmbH, Munich

The Malm aquifer is one of the most important deep groundwater aquifers in Germany and is used for geothermal exploration. Detailed knowledge of the hydrochemical conditions of the deep groundwater is crucial for the technical design of geothermal power plants. The objective of this study was a hydrogeochemical mapping of the groundwaters and of the gas phase in the Malm aquifer in the Bavarian Molasse Basin.

The hydrochemical conditions in the Malm aquifer can be characterized as the result of meteoric waters interacting with the carbonates that make up the Malm aquifer. The hydrochemical analysis are in agreement to the lithostratigraphy. This also implies slow groundwater movement in the Malm aquifer to the basin center. Simulations of the Malm water generation confirm the infiltration of overlaying formations in the central basin and suggest an influence of a predominantly dolomitic aquifer. There are hydrochemical exceptions in some regions of the Molasse Basin, where an influence of oilfield waters, waters with high mineralisation or cristalline influenced waters can be observed.

The particle concentration of the Malm water was studied at two sites in the central basin. The elementary concentration indicates that new formed particles are present as well as original components. Furthermore, abrasion of technical material was observed. The particle composition depends strongly on the chemical composition and character of the thermal water. An average value of 73 ± 145 NmL/L was determined for the total gas concentration in the Malm water. The main component of the gas phase is carbon dioxide (CO_2). Moreover the gas contains nitrogen (N_2), methane (CH_4) and hydrogen sulfide (H_2S). The average degassing pressure is 5 to 15 bar in the central basin. The locally changing hydrochemical character is also reflected by the sulfur distribution. The highest sulfide concentrations in water and H_2S-concentrations in the gas phase were measured in the southern central part of the Molasse Basin. Continuously decreasing sulfate concentrations from the basin margin to the central basin imply increasing reductive conditions to the central part of the Molasse Basin. The H_2S concentrations in the gasphase show an average value of 10.4±48.8 µmol/L. Maximum concentrations were documented in the South East of Munich. Regional variations can be observed.

C. Mayrhofer

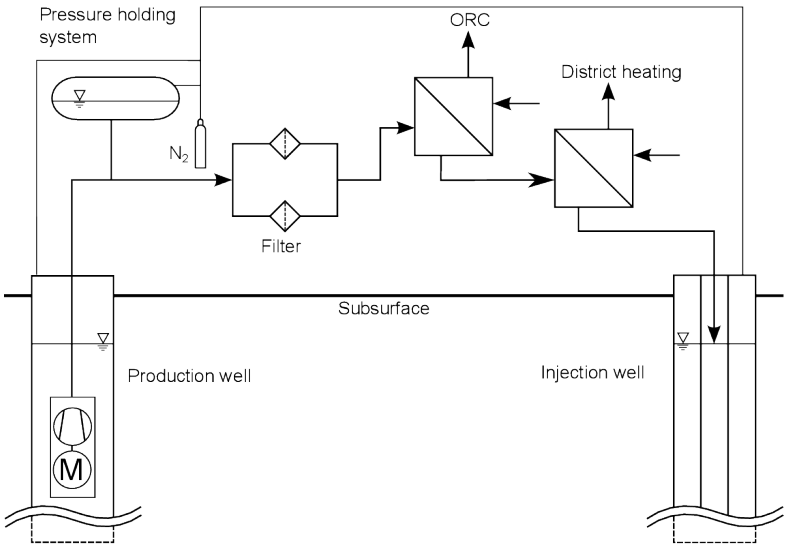


Schematic of the processes relevant for the hydrochemical characteristics of the thermal water in the Malm aquifer

Minimizing Risks for Geothermal Power Plants

Funding: BMU
Cooperation: SWM Services GmbH, Munich

Following the geothermal power plant Unterhaching and several facilities for distributed heating, a number of ambitious project have been launched to produce electrical power from geothermal energy. As noted previously, the hydraulic and hydrochemical conditions at the different sites are extremely heterogeneous and hard to predict. This affects the design of the facilities, long term operation, and raises economic issues



Schematic of a geothermal power plant

In comparison to district heating facilities geothermal power plants usually are only effective at high volume rates and high temperatures. Thus, even small changes of hydrochemical equilibria may result in serious scalings in tubings and heat exchangers. Degassing of the thermal water is a major issue as the pressure required at the well head is indirectly correlated to the efficiency of the power plant. Precipitation of small particles during production might lead to clogging in the heat exchangers and will affect the hydraulics of the reinjection wells badly.

Within a BMU funded project the scientific base for a cost effective exploration and operation of geothermal power plants are addressed using the SWM power plant in Sauerlach as an example.

A gas monitoring of the thermal water has been designed using a micro-GC to record the short term, medium term and long term variability of the gas concentration in thermal water. With this data the prediction of degassing in the heat exchangers and tubings can be predicted much more reliable.

Further work addresses colloid formation during production and an optimized filter design. Here, the experience at the different sites range from "no problem at all" to a requirement of daily backflush of the filters due to large particles accumulating. As geochemical models suggest that the formation of precipitates, either as scaling or as particles, are correlated to the gas composition and gas concentration of the thermal water, these effects have to be evaluated in together.

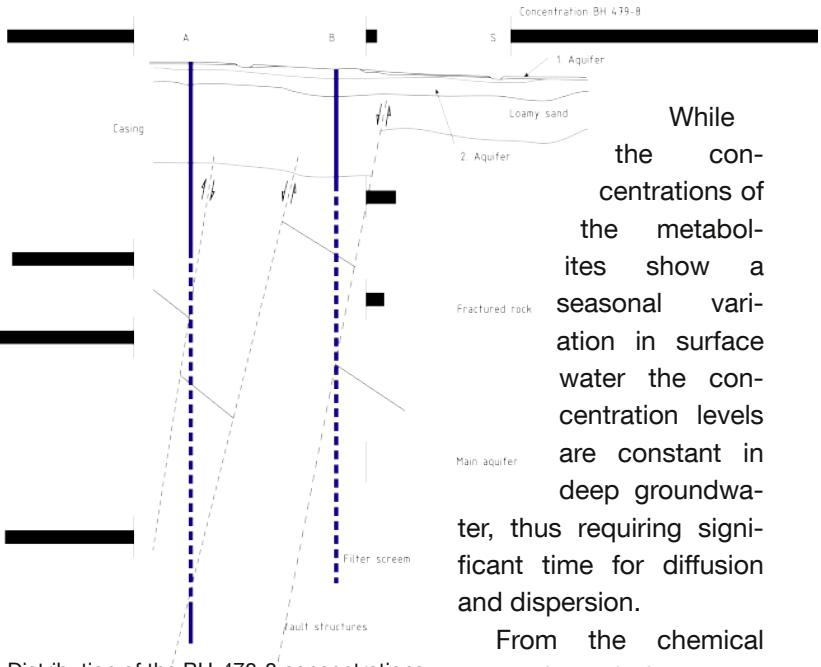
The field tests will be accompagnied by experiments in an autoclave, where the kinetics of individual processes can be studied.
Moritz Herbrich

Persistent organic trace substances in deep groundwater

Funding: IWC

Recent advances in analytical instrumentation offer exciting new possibilities for groundwater monitoring. With LC-MS/MS persistent organic trace substances can be identified and quantified in concentration levels down to several ng/L. This has led to a number of "first time" detections of organic trace substances, even in deep ground water aquifers. Within the current framework of directives for mineral water, the detection of organic trace substances is usually interpreted as a failure of the top layers protecting the source of the mineral water against all risks of pollution. This interpretation connects the detection of organic trace substances to a direct contamination from the surface, thus reducing the hydrogeological, hydrochemical and microbiological description of the catchment and source of the mineral water expertise to a binary technical definition. It is evident that the groundwater withdrawn from a well has to be recharged somehow. At first recharge takes place in the immediate surrounding of the well with a certain amount of mixing with groundwater from higher stratums and, on the long run, with precipitation. All substances with similar transport properties as water itself are expected to show up in deep groundwater sooner or later.

At a small catchment metabolites of the pesticide metazachlor were detected. As non-relevant metabolites they do not have any toxic or ecotoxicological effects (see Fig.). Isotopic measurements indicate that the groundwater in the deeper aquifer is at least 5 to 15 years old.



Distribution of the BH-478-8 concentrations in a fractured aquifer

While the concentrations of the metabolites show a seasonal variation in surface water the concentration levels are constant in deep groundwater, thus requiring significant time for diffusion and dispersion.

From the chemical properties of the metabolites, retardation along the flow path is negligible. In this sense the metabolites are comparable to Tritium, which is an accepted tracer for groundwater. It is important to accept, that the identification of trace substances in groundwater does not imply a detoriation of the top layers and that there is no geological protection against the propagation of water and substances with similar transport properties.

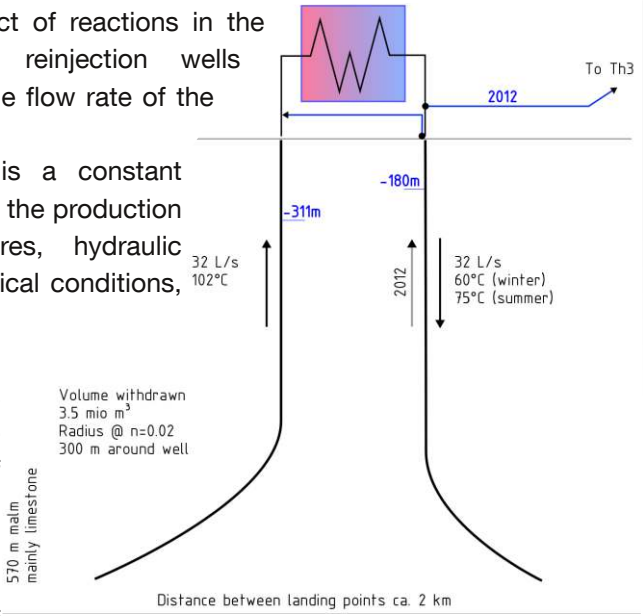
T. Baumann

A Push-Pull Tracer Test at a Geothermal Well

Funding: IWC
Cooperation: IEP GmbH, Pullach; Erdwerk GmbH, Munich; Appl. Geosciences, Univ. Göttingen

Long term operation of geothermal facilities is strongly depending on the aquifer properties. These, however, are hard to assess because the aquifer is some thousand meters below ground surface and sample cores from the exploration are usually not feasible. The aquifer properties, and their possible changes in the cause of the operation, are relevant for an effective recovery of the heat energy stored in the rock matrix and the energy required for reinjection of the thermal water. The impact of reactions in the surrounding of reinjection wells increases with the flow rate of the facility.

While there is a constant flow of data from the production well (temperatures, hydraulic data, hydrochemical conditions, gas composition), not even the temperatures in the immediate surrounding of the reinjection well are known. The long-term performance of the geothermal facility is assessed mainly based on hydraulic models. There are, however, indications that the general assumptions have to be reconsidered, as the increasing viscosity of the cooled thermal water should cause an increase of the reinjection pressures. In contrast monitoring data shows constant and even decreasing reinjection pressures. The reason is not yet clear, but hydrochemical processes certainly contribute to this compensation in reactive aquifer materials.



Schematic of the Pullach geothermal facility

The Pullach geothermal district heating plant has been in operation since 2006. When the facility was extended with a third geothermal well (Th3) in 2011 a unique scientific oppurtunity arised: For the first time the reinjected water from a geothermal well in full operation could be withdrawn to validate our hypotheses about the thermal, hydraulic, and hydrochemical conditions in the vicinity of the reinjection well.

To make the most out of the reverted flow, a series of tracer pulses were added to the reinjected thermal water before the reinjection well was shut down. These tracers include conservative tracers, slightly sorbing tracers, a partioning tracer, and a thermal tracer in cooperation with Martin Sauter's group at the University of Göttingen.

Currently the tracers rest at distances between 20 and 180 m from the reinjection well. As soon as production resumes (march/April 2012) a detailed monitoring programme will be put into effect to recored the tracer recovery curves, temperatures and hydrochemical conditions.

S. Sailer, M. Lafogler

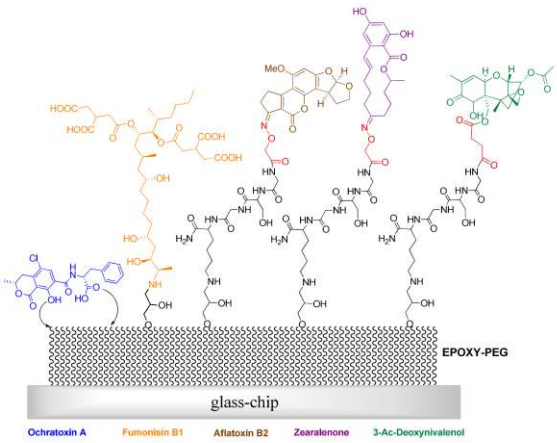
Bioanalytics (Apl. Prof. Dr. D. Knopp)

Hapten Microarray-based Screening of Mycotoxins in Cereals

Funding: AiF (FEI) (Allianz Industrie Forschung), Verband Deutscher Mühlen
Cooperation: LS Hygiene u. Technologie der Milch, LMU, Prof. Märtlbauer, Dr. Dietrich

Mycotoxins, even when present in low concentrations, represent a significant hazard to human health and more than 90 countries worldwide have directed considerable efforts to introduce, regulate and standardize the levels of mycotoxins in food and animal feed. Mycotoxins are secondary metabolites produced by fungi on agricultural commodities and, dependent on the nature of the specific compound, can be acute toxic, immunosuppressive, mutagenic, teratogenic, and carcinogenic when ingested by human beings and animals. The most important mycotoxins in cereals are ochratoxin A, deoxynivalenol, aflatoxins, zearalenone, fumonisins and T-2/HT-2. The common analytical procedure for the detection and quantification of these mycotoxins in several food commodities usually consists of HPLC/UV-Vis, fluorescence, and/or mass spectrometry. Immunoaffinity clean-up (IAC), as a variant of solid phase extraction, has been widely developed and turned up for several foodstuffs as a powerful pre-treatment method for chromatographic analysis to remove matrix constituents which do interfere with the detection. Although very selective, IAC cartridges are quite expensive and usually not suitable for column recycling. Competitive enzyme-linked immunosorbent assays are a viable alternative to the many HPLC-based procedures, since the food extracts can be analyzed with little or no pre-treatment. However, they do not allow multianalyte testing, generally. Therefore, in this project, the previously developed MCR3 and biochips are tested for the rapid determination of multiple mycotoxins in cereals. In detail, coupleable mycotoxin derivatives are synthesized and then immobilized on special PEGylated glass chips yielding a hapten-microarray. The immunological determination takes place in a flow chamber and the chemiluminescence readout is performed by a CCD camera placed on the top.

In the first part of the project, a set of mycotoxin derivatives was synthesized and a variety of methods tested for glass slide functionalization. Dose-response curves were constructed with different kinds of cereal extracts. Also, the robustness of the biochip was investigated and measures taken against loss of the signal intensity along several regeneration cycles, e.g., by using different blocking solutions. Further efforts were devoted to initial testing of several extraction methods for obtaining high recovery of mycotoxins with simultaneous undisturbed determination and the generation of a highly affine monoclonal ochratoxin A antibody.



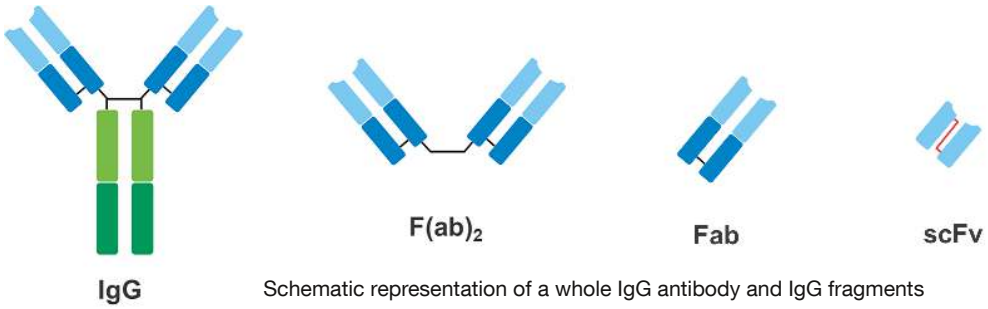
Schematic of mycotoxins bound covalently to the microarray chip

S. Oswald

Recombinant Antibodies Against Benzo[a]pyrene and Insights Into Paratope-epitope Interactions by X-ray Crystallography

Funding: BMBF
Cooperation: Martin-Luther University Halle-Wittenberg, Quo data GmbH Dresden, University of Guelph, Canada

Polycyclic aromatic hydrocarbons (PAHs) are formed during incomplete combustion of organic compounds. Because of their high toxicity a limit value was set by the European Commission (Council Directive 98/83/EC) for Benzo[a]pyrene (B[a]P) of 10 ng/L in drinking water. Sensitive and reliable analytical methods are needed to detect B[a]P at this very low concentration.



Schematic representation of a whole IgG antibody and IgG fragments

In the past, we reported on the development of a highly sensitive indirect competitive ELISA for the detection of B[a]P in potable water. With the best antibody (clone 22F12) an LOD of 24 ng/L was obtained. With further optimization of the ELISA procedure using a 3-Fluoranthenyl-BSA coating conjugate and a poly-HRP labelled secondary antibody, LODs could be reduced below 20 ng/L for two monoclonal antibodies (18 ng/L for clone 22F12 and 19 ng/L for clone 5E11). But still antibodies with a higher affinity to B[a]P are needed to reach the limit value of 10 ng/L.

Recombinant antibodies (scFv) were produced based on the genetic information of three highly affine monoclonal antibodies, but with the scFvs produced yet no improvement in sensitivity could be obtained. As higher sensitivity may be achieved by a genetic manipulation of the antigen binding site, detailed information about antigen binding is to be gained using X-ray crystallography. For that purpose, Fab fragments have been produced by enzymatic digestion of monoclonal antibody 22F12. Crystallization will have to be optimized for the B[a]P-antibody complex in order to obtain crystals suitable for X-ray crystallography.

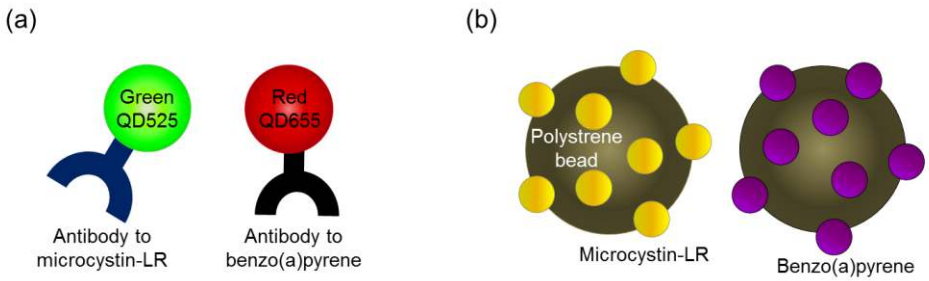
X.Y.Z. Karsunke, M. Pschenitza

Multiplexed Microsphere-based Assay of Environmental Contaminants Using Flow Cytometric Detection of Quantum Dots(QDs)/Antibody Probes

Funding: DAAD, IWC
Cooperation: Gwangju Institute of Science and Technology, Republic of Korea

Suspension assays (bead-based assays) using encoded microparticles have become important to flow cytometry because of the ease of antibody/antigen conjugation and the possibility that particles can be used to detect targets too small (e.g. chemicals) to generate a significant scattered light signal. Encoded beads are already in use commercially, mainly for assays that require multiplexing in small sample volumes. They have been shown to have sensitivities comparable to both ELISAs and microarrays. For evaluation, optical detection methods (combination of light scattering and fluorescence) have emerged as the standard for flow cytometry. A new generation of fluorescent labels, colloidal semiconductor nanocrystals (also referred to as quantum dots (QDs) have attracted a great deal of interest in the biosensing community after Nie et al. and Alivisatos et al. described their first description in a biological context in 1998. For example, with their broad absorption spectra, QDs could simplify the experimental setups with single excitation source and no FRET conjugates.

One possible application area is labelling of assay reagents, which is studied in this project. In detail, QD/antibody (QD/Ab) detection probes (prepared with benzo[a]pyrene (B[a]P) and microcystin-LR antibodies) and polystyrene bead (PB) capture probes functionalized with either B[a]P or microcystin-LR, were prepared and used for the immunological recognition of the target analytes. Two commercially available QDs (green and red) were used to obtain detection probes. Different capture probes were prepared by using commercially available Streptavidin coated PB and biotinylated target analyte-derivatives. Analysis was performed with Cell Lab Quanta SC flow cytometer. For evaluation, the electronic volume and side-scattered light are used to obtain information about particle size, i.e., to differentiate between single beads and QD/Ab/B[a]P/bead aggregates; (QDs) fluorescence (two fluorescence channels) is used to quantify fluorescently labeled aggregates and for calculation of the B[a]P and microcystin-LR concentration in different water types like tap water, bottled water, and surface water samples.



Schematic drawing of (a) QD/Ab detection probes and
(b) PB/target analyte (B[a]P or microcystin-LR) capture probes site

Hye-Weon Yu

Highly Sensitive and Specific Determination of Hg(II) with an ELISA Based on a Novel Monoclonal Antibody

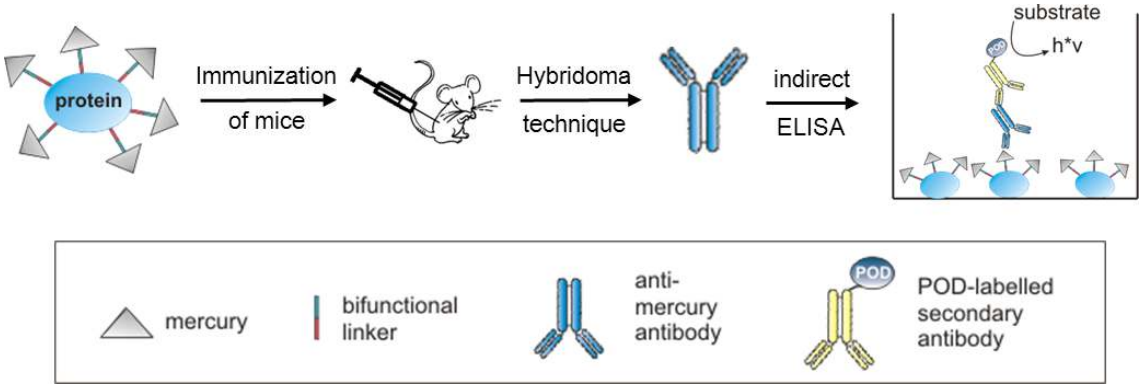
Funding: IWC
Collaboration: College of Chemistry, Sichuan University, Chengdu and College of Chemistry, Soochow University, Souzhou, China

Rising emission rates of mercury into the environment pose a worldwide thread to human health. Major source of mercury emission is the burning of fossil fuels, among which coal contains by far the highest mercury impurities. The WHO recommends a limit value of 6 µg/L for inorganic mercury in water and in Germany the limit value set by the European Commission is 1 µg/L for mercury in drinking water. Fast and sensitive analytical methods are needed for monitoring the presence of Hg(II) at very low concentrations in several matrices.

In cooperation with the group of Prof. A. Deng (Soochow University, Suzhou, China) an indirect competitive ELISA with high sensitivity and selectivity for mercury(II) was developed. The generation of monoclonal antibodies was carried out by immunization of mice with a mercury-protein-conjugate using a new bifunctional linker. Monoclonal antibodies were then produced using hybridoma technique. With the most sensitive antibody an indirect ELISA was developed showing very high sensitivity with the lowest values for IC50 and LOD obtained so far in anti-mercury(II)-ELISAs. Low cross-reactivity was found for the linker and the mercury-linker complex and no reaction at all with any of the tested metal ions and different anions, showing the high selectivity of the assay.

Measurement of different spiked real samples showed acceptable recovery rates and were very comparable to atom fluorescence spectroscopy.

M. Pschenitza



Antibody generation and assay development for an anti-mercury(II) ELISA.

Applied Laser Spectroscopy (Univ.-Prof. Dr. C. Haisch)

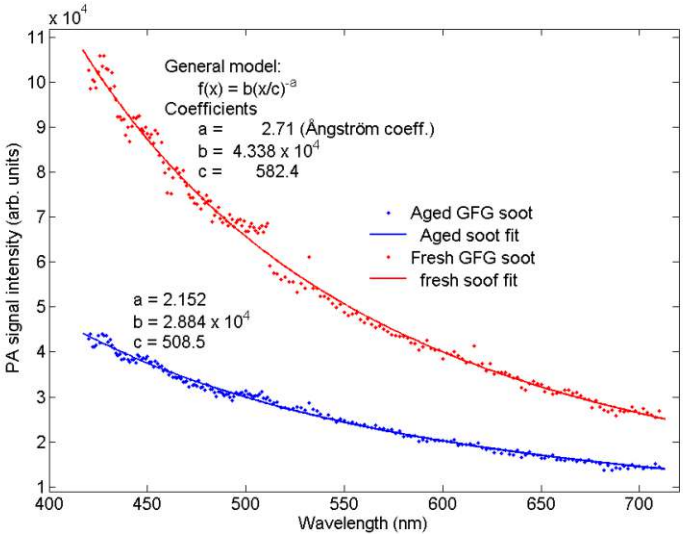
Improved Performance of the Photoacoustic Aerosol Spectrometer

Funding: IWC

When photons are absorbed by matter, the photon energy is transferred into a local heating followed by thermal expansion resulting in the generation of a sound wave. This light matter interaction is called photoacoustic (PA) process. Usually modulated light, generated by a continuous wave (cw) laser diode, is used as the phonon source. The disadvantages of this method are the limited wavelength tuneability of the laser diodes and the fact that there are gaps in the available wavelength spectrum.

Our new Photoacoustic Aerosol Spectrometer is based on a frequency tripled Q-switched Nd:YAG laser generating a pulse energy of ca. 50 mJ at 355 nm. The short pulse width of about 5 ns results in an intensity of 10 MW allowing the high efficient pumping of a nonlinear Optical Parametrical Oscillator (OPO). The OPO is generating two light beams simultaneously, the signal beam (410 nm – 710 nm) and the idler beam (710 nm-2600 nm). Both beams and a part of the 355 nm pump light are passed through three individual photoacoustic cells. Inside these cells the photo acoustical sound signals are generated by aerosols interacting with the light beams and detected by microphones. The amplified microphone signals, the pulse energy of the light beams and the particle number measured by a condensation particle counter (CPC) are digitized and stored simultaneously for each wavelength selected for the scan. A Labview program is used to handle the measurement process and the data storage.

The performance of the spectrometer was shown using different kinds of particles. The absorption spectrum of soot particles is following an exponential law defined by the so called angstrom coefficient. Our measurements fit to the exponential decay with a correlation factor of better than 99%. These measurements demonstrate the usability of the spectrometer as a device for spectral absorption measurements. Fine adjustment of the optical parameters and data evaluation increased the sensitivity to 1 Mm^{-1}.



Absorption spectra for fresh (<1 s) and aged (~50 s) spark-generated soot

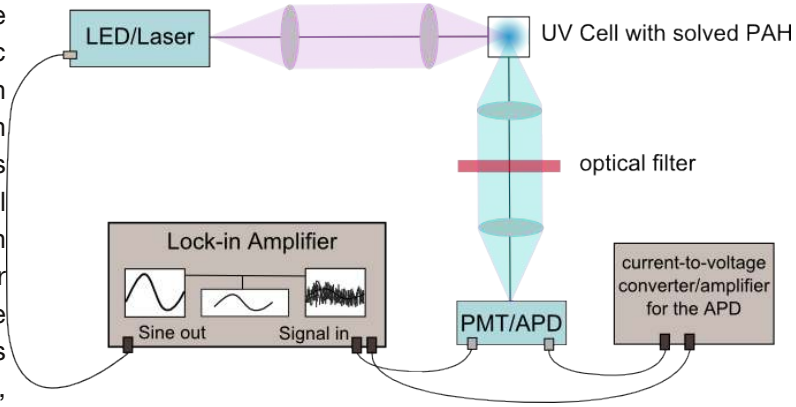
P. Menzenbach

LED-Induced Fluorescence Spectroscopy for Water Analysis

Funding: Hydrometer GmbH, Nürnberg

One of the most widespread organic pollutants are polycyclic aromatic hydrocarbons (PAHs). Some PAHs are extremely toxic. A detection system for drinking water could prevent contamination of humans with these pollutants. Most PAHs exhibit a strong fluorescence which can be exploited for a sensitive analysis. Fluorescence spectroscopy is a sensitive and often used method for the detection of organic compounds. Common excitation sources are xenon arc- or mercury vapour lamps and nitrogen lasers. They all emit in the UV/VIS range. In this range, the molar absorption coefficient of the fluorescence has its maximum. In recent years, also low-priced LEDs appeared on the market, which emit light in the UV and blue range. LEDs are non-thermal emitters featuring narrow emission band widths. These properties make LEDs efficient light sources for discrete excitation applications. Fast modulation of the LED (up to 100 MHz) makes it possible to use lock-in detection to recover signals with a low signal-to-noise ratio. The low price, the long lifetime and the small size allows for the construction of mobile detector systems.

The aim of this project is to develop such a simple and compact detector system and to evaluate its sensitivity. Besides the selection and application of an UV-LED, the main part of the research is devoted to the construction of a low-cost light detector. Low concentrations of the fluorophores and therefore low light intensities demand a highly-sensitive detection system. A high spectral sensitivity in the UV/VIS range, low noise and a high gain are the main requirements for a fluorescence detector. The standard for light detection is the photomultiplier tube (PMT). PMTs combine low noise and a high gain up to 106. A low-cost alternative is the avalanche photodiode (APD). An avalanche photodiode uses the avalanche effect to amplify the signal by a gain of 103. Combined to a high-performance electronic amplifier with an electromagnetic shielding to prevent noise amplification, it is possible to build a highly-sensitive light detector. Analog-to-digital conversion is carried out by means of a commercial USB-based sound card, a low priced, nevertheless high-performance AD-converter. The combination with software-based lock-in data treatment makes allows for sensitive detection in the presence of a significant radiation background. The detection system is powered by batteries to provide the required mobility.



Experimental setup of the LED-based fluorescence monitor

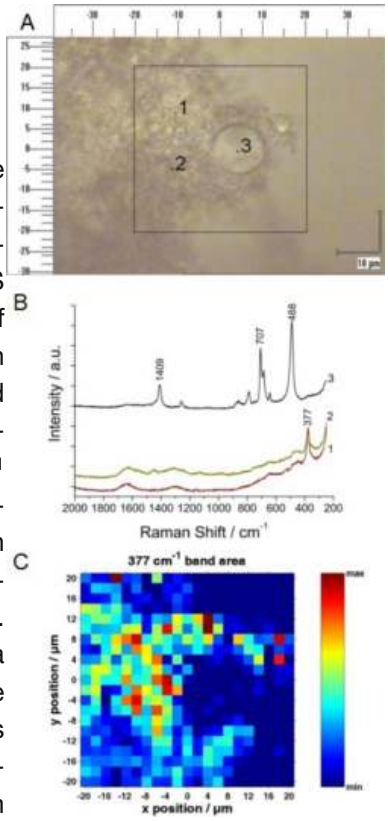
C. Berger

Iron Precipitation in Biofilms Characterized by Raman Microscopy

Funding: DFG
Cooperation: Institute of Water Quality Control, TU Munich

Biofilms are interface associated heterogeneous systems consisting of microbial cells which are embedded in a gel-like matrix of extracellular polymeric substances (EPS). EPS are biopolymers such as polysaccharides, proteins, nucleic acids, lipids, and humic-like substances. Formation of 3D-EPS framework allows cells to survive in diverse environments. The mechanical properties of biofilms and in particular their strength/stability is of importance for biofilm reactors as well as for the removal of undesired biofilms in cases of biofouling/biocorrosion. The beneficial effect of divalent cations on the biofilm strength is well known. The cations such as Ca2+ can induce the cross-linking of different polymer molecules as well as different part of the same polymer chain, e.g. via binding to G-G alginate residues. (Choupta et al., 2000, Körstgen et al. 2001). Positive stabilizing effect was also shown for Fe applied during the biofilm cultivation (Möhle et al. 2007), however the form of iron in biofilm was not clear. Here Raman Microscopy (RM), which is a non-destructive technique for chemical analysis can be employed for the characterization of iron compounds precipitated/imbedded in biofilm matrices.

We observed increased stability of biofilms cultivated with the addition of Fe^{2+} compared with biofilms grown at similar nutrient and flow conditions, but in the absence of Fe^{2+}. Figures A and B illustrate the optical microscope image and the corresponding Raman spectra of different biofilm constituents, such as aggregates and protozoa, obtained from the multispecies biofilm. Aggregates are microorganisms embedded in an EPS matrix. Typical spectra of the aggregates (1 and 2 in Fig. B) show two broad bands of humic-like substances around 1630 cm^{-1} and 1320 cm^{-1}. The prominent band at 377 cm^{-1} can be assigned to largely hydrated iron oxide FeO(OH). This compound causes a light orange color of the analyzed biofilm and is supposed to be the oxidation product of Fe^{2+} from the nutrients used upon biofilm cultivation (incl. $FeSO_4$).



Microscopic image (A), SERS spectra of three different positions (B), and SERS map (C) of a biofilm.

We found that the band assigned to FeO(OH), can be a suitable biomass marker of biofilm grown in the presence of Fe^{2+} (Fig. C). Analysis of biofilms at initial growth phase (3 days old) with new Raman system LabRAM HR (spectra from 50 cm^{-1}) revealed the bands at 250, 378, 526 and 647 cm^{-1} that allowed us to identify the iron precipitate in biofilms as lepidocrocite.

In our further study we will focus on the correlations between iron precipitation/accumulation and physic-chemical properties of different biofilms and the interactions of different iron phases with biofilm matrices .

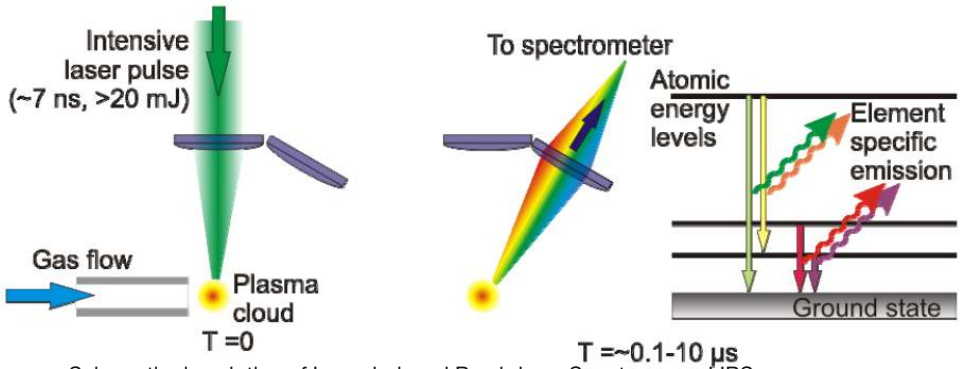
N. P. Ivleva

Detection of Contamination in Biogas Using Laser Induced Breakdown Spectroscopy

Funding: EU (European Union)
Cooperation: Italian Agency for New Technologies, Energy and Sustainable Economic Development, Italy; TUBITAK Marmara Research Centre, Turkey; University of Genoa - DICAT department, Italy; Royal Institute of Technology KTH, Sweden; OVM-ICCPET Institute, Romania; Joint Research Centre JRC, Belgium

The interest in alternative energy sources has increased in recent years. In this context, the European Union funded a project aiming for the use of biogas as an energy source for high temperature fuel cells. Especially, Molten Carbonate Fuel Cells (MCFC) are promising regarding their efficiency and environmental aspects. These cells gain energy by transformation of hydrogen which is produced by reformation of the main component of biogas methane. Depending on the origin of the biogas, the composition can vary and contains impurities such as sulfur compounds, halogenated hydrocarbons, and siloxanes. These contaminants cause undesired reactions at the anode and cathode, which reduce efficiency and lifetime of the cell. In this project, we are responsible for the development of the continuously monitoring of contamination in biogas by laser induced breakdown spectroscopy (LIBS).

The detection system is based on laser induced breakdown spectroscopy (LIBS). LIBS is atomic emission spectroscopy on a plasma spark ignited by an intense focused laser pulse. The emitted light is element specific, and the concentration relates the emission intensity (see fig. 1). For the measurement, the sample gas is flushed through a gas chamber in which the laser is focused from one side, while the light signal is detected rectangular and transmitted by an optical fiber to the spectrometer. For the future applications a spectrometer was bought, which has two different light entrances that allows combining LIBS and Raman spectroscopy.



Schematic description of Laser-induced Breakdown Spectroscopy LIBS on gases

The advantage of the combination of LIBS and Raman spectroscopy is to get atomic and molecular information with high temporal resolution and for a wide range of gas compounds and concentrations.

K. Schwarzmeier

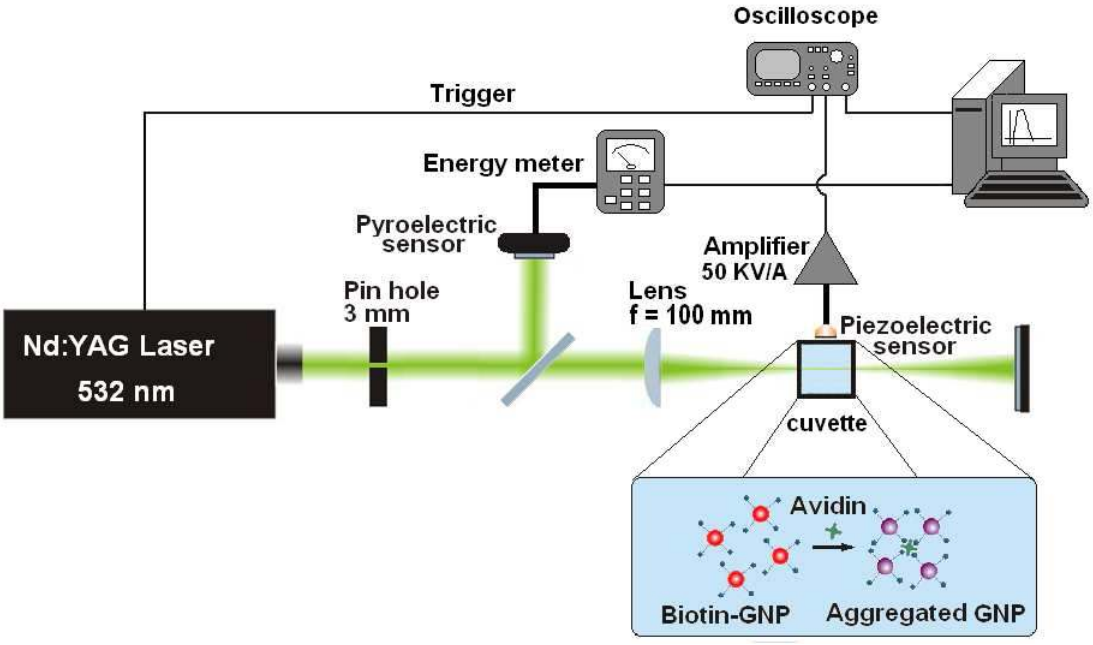
Gold Nanoparticles as Analytical Tool

Funding: IWC; China Scholarship Council

Gold nanoparticles (GNP) have attracted enormous attention for biosensor and bioassay in the past decades. A common sensing mechanism is based on aggregation caused by binding between target and receptor-conjugated GNP, which leads to a colour change of GNP suspension. The colour change can be noticed by naked eyes or can be detected by a UV-vis spectrometer. In this work we present a more sensitive tool to monitor GNP aggregation. This tool is based of measurement of PA signal generated by laser-induced nanobubbles(PA-LINB). The approach can be employed for a wide variety of biosensing applications. We are optimistic that it can also be transformed to plasmonic surface structures.

We found the amplitude of PA-LINB is strong dependent on the GNP size, which can be used for detecting GNPs aggregation. Meanwhile, Pb^{2+} is wildly considered as one of highly toxic heavy metal ions. The maximum contamination level of lead in drinking water is defined by U.S. Environmental Protection Agency (EPA) 75nM. Hence a method to improve colorimetric detection of Pb^{2+} has been developed based on PA-LINB, which can combine the advantages of colorimetric arrays and the high sensitivity of PA-LINA in detecting aggregation. The limit of detection of Pb2+can arrive as low as 8 nM. Further work will be devoted to new analytical applications of this non-linear photoacoustic effect observed on plasmonic nanostructures.

X. J. Liu



Example for the application of Au nanoparticles as probe for biomolecule detection

ComPAS: A Combined Photoacoustic Monitoring System for Soot and NO_2 in Raw Engine Exhaust

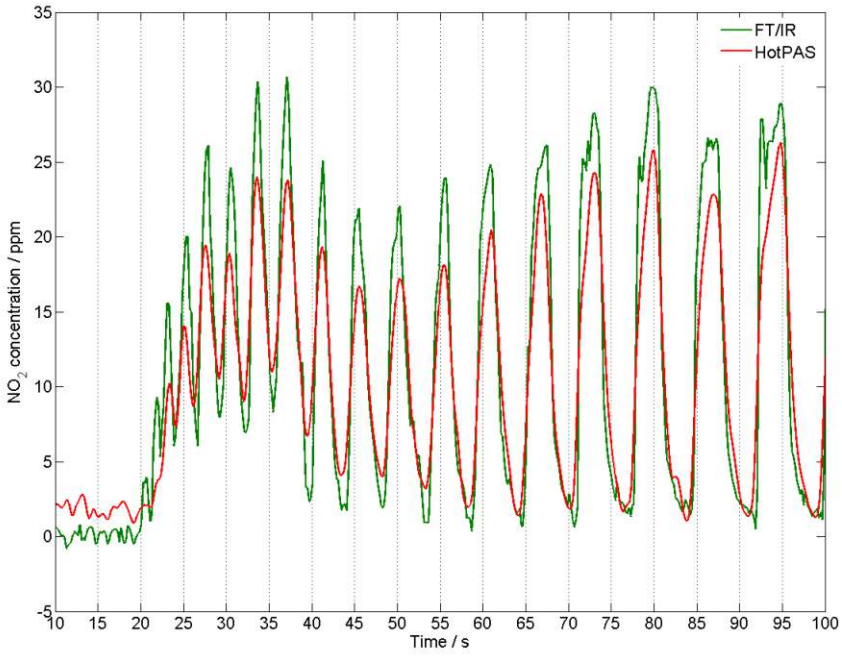
Funding: AVL, Graz

Based on the very successful photoacoustic soot sensor, whose commercial realization is sold more than 600 times all over the world, combined exhaust gas monitoring system is currently developed. The design of the PA cell was modified in a way that measurements up to a temperature of 80 °C are possible, thus allowing measurements directly in raw exhaust gas. While soot is quantified at an optical wavelength of 806 nm, NO_2 is detected at 532 nm.

A key feature of the new design (see Figure) is the new instrument is the fact that the two components are measured in parallel, without filtration of the gas for the NO_2 analysis. A gas filtration, which is common for current standard instrumentation, induces artifacts by chemical reactions of the NO with soot particles deposited on the filter surface. The current instrument features detection limits for soot of 1.2 µg m^{-3} and 0.6 ppm for NO_2. Temporal resolution could be improved to below 1 s, owing to the new cell design.

The next development step will be the extension for further gas components such as NO and N_2O. These gases are accessible only in the IR spectral region, which requires for a different optical setup and new PA cell design.

C. Haisch



Comparison of the temporal resolution of the new ComPAS system and a conventional FT/IR spectrometer

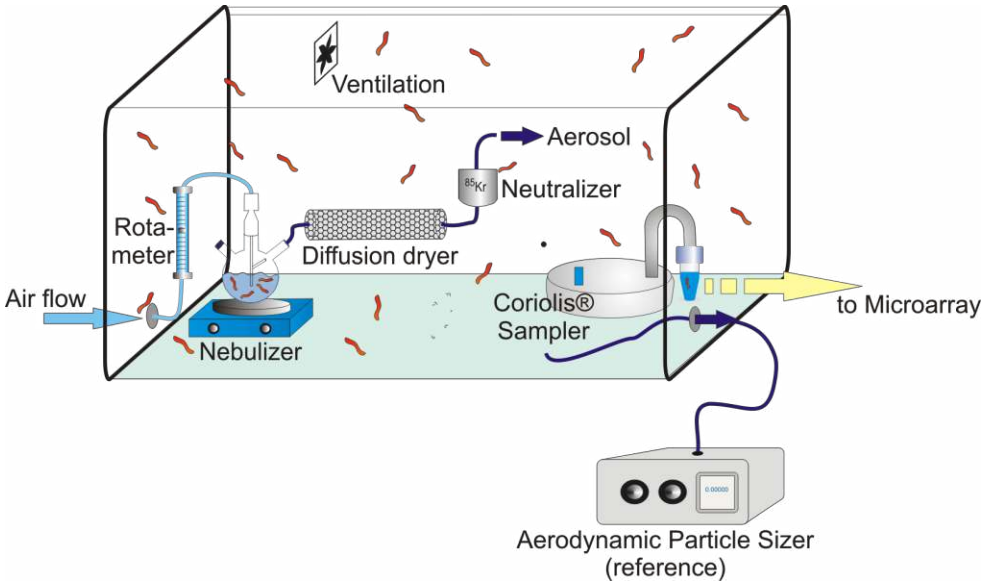
Microarray Readout by Surface-Enhanced Raman Scattering (SERS) for Bioaerosol Monitoring

Funding: IWC

Bacterial contamination of indoor air is a serious threat to human health. Pathogenic germs can be transferred from liquid solutions to aerosol phase for instance when the water forms an aerosol like in showers, air conditions, or spas. Existing analytical instruments for the assessment of indoor air quality assessment and contamination monitoring are mostly time consuming as they generally require for a cultivation step. The need of a rapid, sensitive and selective detection method of bioaerosols is evident.

We developed a new microarray flow-through system for SERS measurements of bioaerosols. This system has been constructed to ideally support the non-destructive in situ analysis of different microorganisms in aerosol environment with a LOD of 222 particles/cm³. The bioaerosols are collected in buffer solution by a commercial portable air sampler (Coriolis µ). Antibodies directed to the desired microorganisms are immobilized on a microarray surface. Following, this detection platform is placed in a flow cell through which the aerosol sampling liquid sample is flushed. Finally, Ag colloids are added SERS substrates and the cells are analysed and quantified.

K. Schwarzmeier, M. Knauer



Experimental setup for controlled production and sampling of bioaerosol with subsequent microarray/SERS detection

Laser-Based Separation (Head: Dr. C. Helmbrecht)

Photophoretic Separation of Hydrocolloids

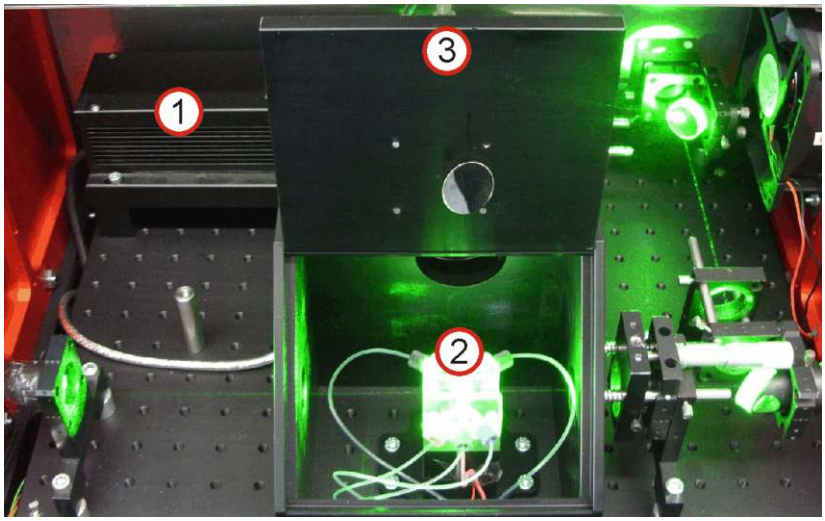
Funding: DFG

The knowledge of particle parameters such as size distribution and chemical properties is essential for the clarification of origin and faith of particles in environmental, geological and chemical processes. Both, physical and chemical characterization simultaneously is often desired but requires elaborate technical instrumentation. The analysis of optical parameters such as absorption and refractive index can be used for chemical identification. The optical manipulation of media leading to migration is termed photophoresis (PP). The application of optical forces on suspensions is a new approach for characterization and separation of colloid matter. The interaction of light with media depends on optical parameters, i.e. photophoresis is capable of fractionating of particles of e.g. same size but different refractive index.

A photophoretic bench-top system was realized and has been tested. A 1.7 W cw-Nd:YAG laser was used as powerful light source. The laser beam was perpendicular to the flow direction of a particle containing liquid. A microfluidic system focuses a colloid beam of ~300 µm width. Particles in the proximity of the laser beam undergo a lateral displacement in the direction of the propagation of the laser beam. The lateral displacement is dependent on the particle properties and is the key of optical separation.

The contact-free separation of in water suspended particles by photophoresis does not require any auxiliary information such as labeling because the generated optical forces are directly dependent on size, refractive index, absorption and shape of the particles. The application of photophoresis as a lable-free separation technique could be beneficial especially for the separation of different microorganisms in suspension.

C. Helmbrecht



The photophoretic bench-top separation system contains a laser source (1), flow-cell (2) and a camera (3, hidden).

Enrichment of Nanoparticle Suspensions by Directional Freezing

Funding: IWC

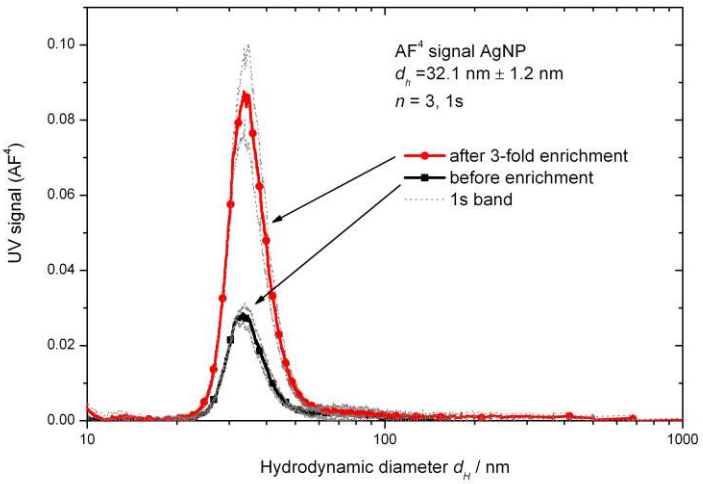
The use of nanoparticles (NP) with tailored optical or chemical properties for the improvement of products ranging from coatings, foodstuff and cosmetics is increasing. Due to use and disposal of such refined products artificially synthesized NP, termed engineered nanoparticles (ENP), are ubiquitously present in the environment. The in-situ detection and discrimination of ENP's at such low concentrations remains a challenging task for state of the art instrumentation. The enrichment of samples prior to analysis would help to penetrate to lower detection limits for nanoparticles.

Directional freezing of water is a new technique for the enrichment of water-suspended particles, e.g. hydrocolloids. When the bottom of a sample compartment containing water is cooled below the freezing point, ice formation starts at the water-wall interface resulting in an ice layer with increasing thickness. Ideally, only water molecules are incorporated to form the ice crystal. In that way, the NP concentration increases in the overhead liquid.

A batch system was designed for the enrichment of suspensions of approx. 15 mL. The base of the sample compartment (glass vial) is attached to a cooling device. The influences of freezing and stirring conditions were studied on suspensions of silver, gold and polystyrene nanoparticles. The fast and precise in-situ determination of particle size distributions of both enriched and natural nanoparticle suspensions was performed by asymmetric flow-field flow fractionation (AF4) equipped with slot-out-let (SOL) technique. The size distributions determined by AF4 were compared to distributions obtained from digital processing of TEM images.

In all experiments the effect of the enrichment process on the nanoparticle dispersions based on the comparison of the size distributions are negligible. Directional freezing is also capable of enrichment of low concentrated dispersions; nanoparticle suspensions with a silver content of 50 ppb were enriched. The laboratory-scale enrichment system is capable of an 8-fold enrichment with typical recoveries of 70%.

C. Helmbrecht



Particle size distribution of silver nanoparticles (AgNP) before (black) and after (red) 3-fold enrichment by directional freezing

Bioseparation and Microarray Technology (Dr. M. Seidel)

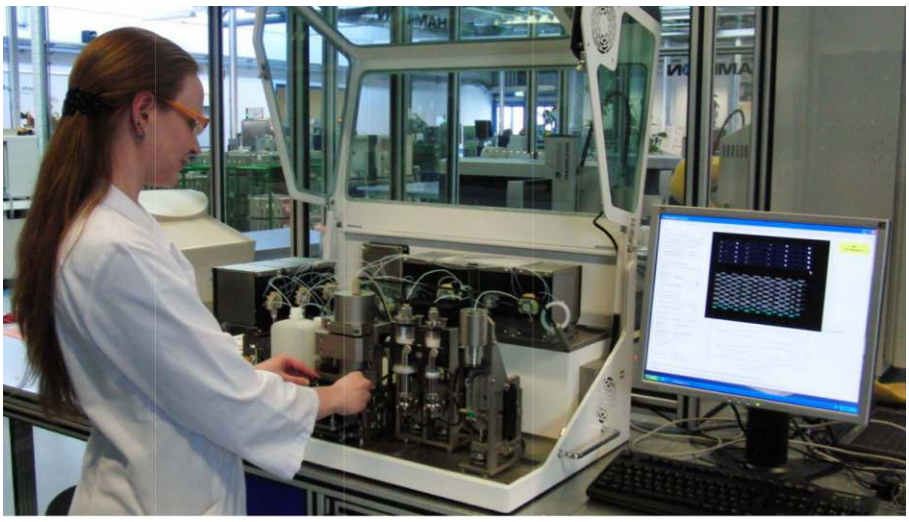
Flow-Through Microarray Chip for Routine Quality Control of Antibiotics in Milk

Funding: Bayerische Forschungsstiftung (Bavarian Research Foundation)
Cooperation: GWK Präzisionstechnik GmbH (Munich)

The objective of this project was the establishment of an instrumentation for automated analyses of 14 antibiotics in milk which can be applied in routine laboratories like milk control labs or dairies. Therefore, parts of the MCR 3 were further developed like the electronic control unit, the software for process control and data processing, as well as the production of the flow-through microarray chips.

The stand-alone platform is now equipped with a SPS control unit and a professional software for the fluidic processing of valves and syringe pumps revealing significant shorter assay times than with the previous process control. The analysis time including chip regeneration could be reduced from nearly 10 minutes down to about 6 minutes. Also, the function of an autosampler is now implementable. These further developments were tested at the institute by characterization of the MCR 3 with calibration curves applying the multianalyte antibiotic immunoassay. Furthermore, a user-friendly interface for robust and automated data evaluation was implemented and tested at our institute. The routine laboratories of the Milchprüfring Bayern (MPR) have tested the final version of the MCR 3 (see Figure) and gave us positive feedback regarding the instrumentation, system performance and data analysis. To summarize, the aims of the project have been achieved at our institute and the further steps of the MCR 3 on its way of commercialization will now be continued by R-biopharm AG, a well-established provider of analytical solutions in the field of food safety and quality control.

K. Wutz



MCR3 in action at the Milchprüfring laboratory in Wolnzach

Biotoxin Microarray

Funding: IWC
Cooperation: Institute of Agri-Food & Land Use, Queen's University Belfast; Robert Koch-Institut, Berlin; Chair for Hygiene and Technology of Milk, LMU Munich

Biotoxins are poisonous substances, which are produced by living organisms like bacteria, plants or animals. The most poisonous substances for humans are the botulinum neurotoxins. Formerly self-made preserved fish or meat could be contaminated with botulinum toxin, but nowadays poisoning with botulinum only indicates a bioterroristic background. Also, other toxins like ricin, saxitoxin (STX) or staphylococcal enterotoxin B (SEB) could be implemented for small scale bioterroristic attacks.

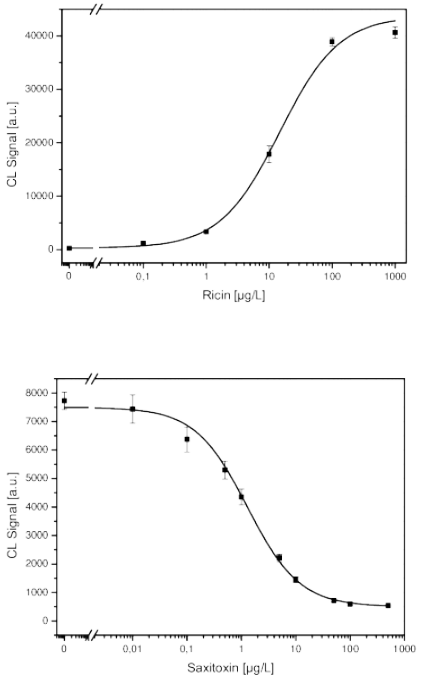
Besides domoic acid and okadaic acid, STX could be found in contaminated seafood. Marine toxins are small molecules, which are produced by microalgae and ingested by shellfish. When humans consume contaminated seafood, they suffer from different poisoning symptoms.

To prevent contamination of water and food, a rapid and sensitive screening method for the simultaneous detection of biotoxins is required. The microarray technology poses a great potential because of the possible multiplex detection of different biotoxins. One application of the microarray will be the detection of biological warfare agents like ricin, SEB and STX and the second application will be the seafood monitoring involving the marine toxins.

Ricin and SEB are high molecular-weight proteotoxins. So the quantification of these biotoxins will be carried out using a sandwich immunoassay. STX being a small molecule can't be detected within a sandwich format. Therefore an anti-idiotypic antibody, which imitates saxitoxin, was developed by Prof. Märtlbauer in order to detect saxitoxin on an antibody microarray format. The limits of detection for ricin (0.1µg/L) and STX (0.3 µg/L) are in the lower µg/L range. The next steps are the fast and sensitive detection of STX, ricin and SEB in parallel.

For the detection of marine toxins an indirect competitive immunoassay was developed. Due to the direct immobilization of the marine toxins on the chip surface, seafood microarrays are regenerable. Therefore only one microarray chip can be used for the calibration and determination of samples. The assay time including the regeneration step takes 18 min. Multi-analyte calibration curves of the marine toxins were generated in buffer with low LODs (1.0 µg/L for DA, 0.8 µg/L for OA and 0.1 µg/L for STX). Real sample measurements as well as spiking experiments in shellfish extracts will complete the characterization of this new application on the MCR3

A. Skola

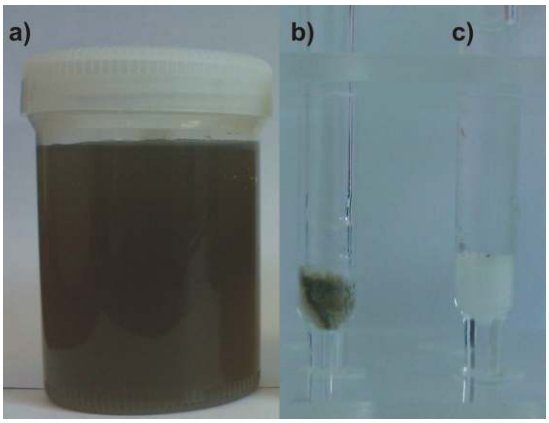


Calibration curves for ricin (above) and saxitoxin (below) quantification on the MCR 3

PATH_2OGENSCAN

Funding: BMBF, China Scholarship Council
Cooperation: State Health Department in Stuttgart, Water Technology Center in Karlsruhe, GWK Präzisionstechnik in Munich, Technion in Israel

Pathogenic organisms and particularly viruses are able to cause diseases in very low concentrations. The aim of this project is the rapid, user-friendly and precise enrichment and quantification of waterborne pathogens and indicator organisms (Norovirus, Adenovirus, Rotavirus, bacteriophages MS2 and PhiX174, E. coli, E. faecalis, L. pneumophila, P. aeruginosa, Cryptosporidium und Giardia).



Concentrated surface water after crossflow ultrafiltration and monolithic affinity filtration

Therefore, we are developing a DNA microarray for multiplexed analysis of relevant pathogens, which should be connectable to a concentration method. The enrichment system should accomplish an effective concentration of pathogens and also the removal of matrix components. Afterwards the nucleic acid of the pre-enriched organisms must be isolated, before amplification in a PCR reaction takes place. Double-stranded PCR product is separated, because only single-strands can hybridize on the DNA microarray to generate a chemiluminescence signal.

A combined enrichment system is developed, containing crossflow ultrafiltration and monolithic affinity filtration to concentrate microorganisms from 10 L to a volume of 1 mL. Spiking experiments with bacteriophage MS2 were performed using two different quantification methods, the qPCR and the new developed DNA microarray. The enrichment system shows good reproducibility and allows enrichment by a factor of 104. For very low concentrations, a high recovery of 97±20% could be observed. The recovery also decreases with increasing concentrations to a stable value of 10% with standard deviations lower than 10%. This effect is due to capacity limitation of the monolithic column. So, further work is done to optimize the columns. The results for the DNA microarray are in good agreement with these, gained by qPCR. Also the enrichment of MS2 from real water samples (surface water) is possible.

Concerning the DNA microarray, it is possible to measure bacteriophage MS2, PhiX174 and Adenovirus. Norovirus will follow within a short time. Furthermore the new MCR3 for DNA application has been comissioned. This device has a completely new fluidic cell unit, which includes a temperature control. The hybridization assay can now be done at higher temperatures to optimize stringency and to reduce cross-hybridization. Further work will be focused on the multiplex measurement of these viruses.

S. Lengger, M. Rieger, L. Pei

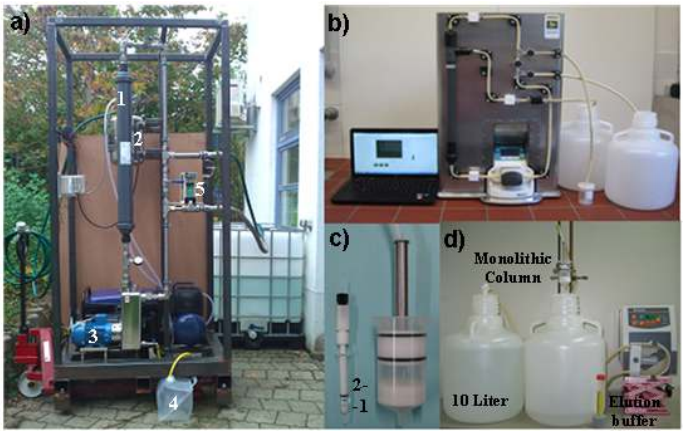
Pathogenic Viruses in Water – Detection, Transport and Elimination

Funding: DFG, China Scholarship Council
Cooperation: Centre of Infectiology and Infection Prevention, University of Bonn; Federal Environment Agency, Berlin; Institute of Groundwater Ecology, Helmholtz Zentrum München; Institut für Siedlungswasserwirtschaft und Abfalltechnik of the Leibniz University, Hannover

Waterborne diseases arise from the contamination of water, either by pathogenic viruses, bacteria or protozoa. In most cases, concentrations of viruses in the ambient environment are lower than detection limits of microbiological assays (e.g. PCR). At the same time, viruses are more infectious than pathogenic bacteria at similar exposures. Based on quantitative microbial risk assessment, WHO proposes there should be typically less than 1 organism per 10^4-10^5 liters in drinking water. To meet these requirements, we proposed the enrichment of viruses from 30 m^3 water to 1 mL, which is compatible to bioanalytical detection methods, like qRT-PCR.

For this purpose, we built up a three-step enrichment system combining two crossflow-ultrafiltration (CUF) steps with monolithic affinity filtration (MAF), as shown in the figure. CUF-Unit 1, having its own power generator on board and being transportable with a truck palette, the system can be set up on site. In dead-end mode, a maximum flow rate of 1724 L/h can be achieved. Enrichment experiments, based on the combination of CUF-Unit 1, CUF-Unit 2 and MAF were carried out. A 30-m^3 water sample was continuously concentrated to a final volume of 1 mL in 20 hours. Including qRT-PCR measurement, the whole analysis procedure was finished within 24 h. In this combination system, every step maintains comparable efficiency when tested separately. With column 2 (Fig. c), 60% MS2 can be concentrated from 10 L tap water within 10 min. Further work will focus on a system, consisting of CUF-Unit 1, positively-charged monolithic column with large diameter and negatively-charged small monolithic column.

The enrichment method was developed



Images of the three step enrichment system

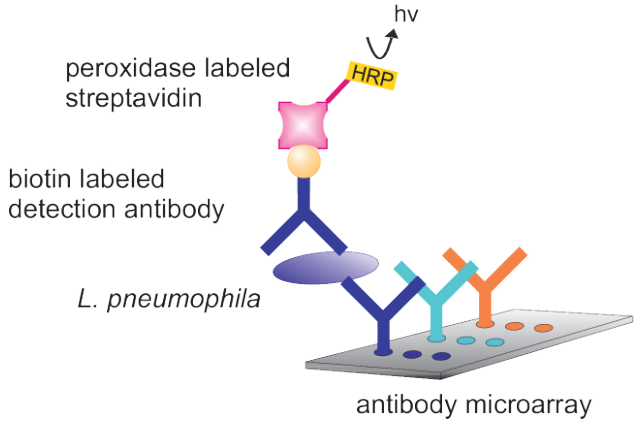
using MS2 bacteriophage as a surrogate. However, in the enrichment of adenovirus and murine noroviruses by MAF, high recovery efficiencies were also achieved (42.4 ± 3.4% and 43.9 ± 2.0%, by N. Hartmann and HC. Selinka, UBA, Berlin). The broad applicability of such combination system promises simultaneous enrichment of various organisms at the same time maintaining ithe diversity of organisms in the original sample in the final 1-mL eluate. This is important for subsequent high-throughput detection methods like microarray technology.

L. Pei, M. Rieger, S. Lengger

Antibody Microarrays for the Detection of *L. pneumophila*

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

Legionella spp. are bacteria occurring ubiquitous in natural and artificial water systems and potentially causing infections for humans. Infections are caused by inhaling contaminated aerosols originating from cooling towers, air conditioners or showers. The periodically analysis of Legionella concentrations for drinking water providers has recently been introduced in the drinking water regulation, leading to an enormous requirement for fast Legionella detection methods. A promising method for fast quantification is the microarray technology. In this project a system for the parallel quantification of the different serogroups of *L. pneumophila* will be developed. Enrichment techniques previous to the detection should improve the detection limit in order to reach defined concentrations. The combined system will be applied for the measurement of water and bioaerosol samples from different distribution systems, potentially giving information about the correlation of Legionella concentration in water and corresponding bioaerosols.



Principle of the sandwich immunoassay site

The detection of *L. pneumophila* is performed with antibody microarrays on an automated readout system. Antibodies, immobilized on a modified glass surface, serve as selective capture molecules. The use of a second antibody allows the formation of a sandwich immunoassay, in case bacteria have been captured on the microarray. The detection is carried out with a horseradish peroxidase catalyzed chemiluminescence reaction. The microarray detection of the most important serogroup (sg 1) has been established and well characterized. Within 67 min *L. pneumophila* can be quantified with a detection limit of $1 \cdot 10^3$-$8 \cdot 10^3$ cells/mL for serogroup 1. In combination with previous enrichment, the detection limit could be improved by a factor of 10. Antibody microarrays could be successfully utilized for the quantification of *L. pneumophila* in bioaerosol samples in a model setup with a detection limit of $4 \cdot 10^3$ cells/m^3. First experiments have been carried out for water and bioaerosol real samples from showers in comparison with other detection methods. In one shower bioaerosol *L. pneumophila* was detected with microarrays, whereas cultivation methods could confirm Legionella contamination in the corresponding shower water. The extension of the microarray platform for the detection of all 15 serogroups has been started. The combination with precedent enrichment techniques will be further optimized to reach concentrations required by law.

V. Langer

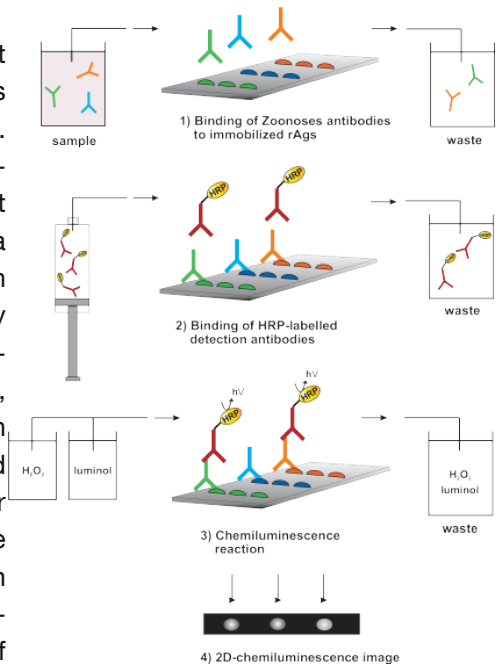
Fast and High-Parallel Detection of *Zoonoses* Antibodies by Means of Chemiluminescence Microarray Immunoassays

Funding: Bayerische Forschungsstiftung (Bavarian Research Foundation)
Cooperation: Mikrogen GmbH (Munich); Chair for Food Hygiene, LMU Munich

Zoonoses are infectious diseases, which can be transmitted from animals, both wild and domestic, to humans. Zoonotic agents are e.g. bacteria, viruses or parasites. In case of porcine meat, the pathogens Campylobacter, Yersinia, Salmonella, Trichinella, Hepatitis E virus, Taenia and Toxoplasma are of great interest for food safety and human health, although only Salmonella and Trichinella are regulated. Thus, multiplexed, simultaneous monitoring of a broad variety of pathogenic microorganisms will help the meat-processing industries to maintain high hygiene standards.

A method for fast and multiplexed detection of Zoonoses antibodies in serum or meat juice samples of pigs for slaughter will be developed, that is, the target is not the determination of microorganisms themselves, but the specific antibodies against them formed by the host. With this approach, information about past and acute infections can be revealed due to the time-dependent existence of different antibodies classes (IgM, IgG, IgA).

To realize this aim, a detection method based on immunoassays (ELISA) in a microarray chip format is used. Recombinant antigens (rAg) are immobilized on functionalized glass slides. The microarray chip is then incubated with serum or meat juice samples. In case of contamination with Zoonoses antibodies, these antibodies bind on the chip surface and can be detected by means of horseradish peroxidase (HRP)-labelled secondary antibodies. Using specific secondary antibodies to IgM, IgG and IgA, discrimination of different antibody classes is also possible. The chemiluminescence readout via CCD-camera is performed on the microarray chip reader platform MCR 3, which had been developed and proved in former projects. The MCR 3 platform allows for automated delivery of all needed reagents and combines the flow-through principle known from flow-injection systems with the microarray technology. With this powerful tool, incubation times can be clearly reduced compared with ELISA test formats performed in titer plates and analysis can be done for a variety of analytes in parallel.



Principle for the detection of zoonoses antibodies on microarrays

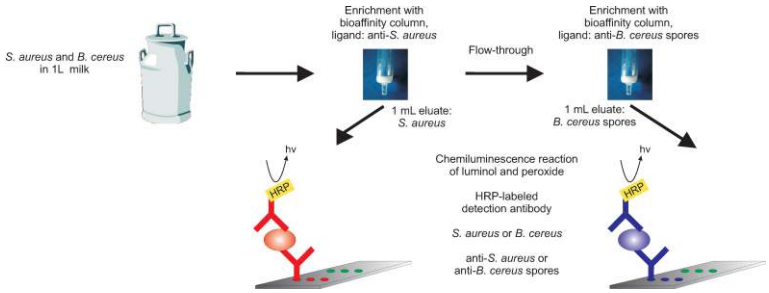
Up to now, we have successfully established a microarray immunoassay for principle studies on the target analyte of IgG antibodies formed against the Hepatitis E virus. Within an assay time of 7 minutes we can detect HEV antibodies in real serum samples. The next steps will be the integration of further antigens on the chip surface and the optimization of the chip regenerability.

K. Wutz

Detection of *Staphylococcus aureus* and *Bacillus cereus* in Milk After Enrichment With Bioaffinity Columns

Funding: AIF/FEI, BMBF
Cooperation: Chair for Hygiene and Technology of Milk, LMU München; Institute for Food Chemistry, University Hamburg; Chair for Fluid Mechanics, Friedrich-Alexander-University Erlangen-Nürnberg

In diary industry the fast identification of contaminants of microorganisms is very important. The major pathogens are *Staphylococcus aureus*, the indicator for hygiene and *Bacillus cereus*, the indicator for decayed food. Together they are responsible for half of all food poisonings. Routinely they are detected with cultivation methods which are very specific and sensitive, but also time and labor intensive. Therefore we are working on a combined analytical separation and detection method, in which the milk sample is prepared for a detection system that can detect the pathogens in a considerable shorter time and quantify several microorganisms in parallel.



Schematic of the rapid quantification of B. cereus and S. aureus

By using the monolithic immunofiltration, microorganisms are concentrated from a volume of 100 mL. Disturbing matrix components are removed and the subsequent detection is facilitated. The stationary phase is a monolithic support, which was developed for the enrichment of microorganisms and which was modified for the use in milk. The surface is designed to have minimal attachment of the milk components. For affinity ligands antibodies against *S. aureus* and *B. cereus* spores are immobilized, which capture the microorganisms in a selective way. After elution the concentrate is measured directly at a chemiluminescence based microarray platform with sandwich-ELISA.

10^3-10^5 B. cereus spores could be enriched in 100 mL PBS buffer or milk. The enrichment in milk was done at 37°C to decrease the back pressures and to solve the matrix components like fats. The microorganisms are concentrated within 15 min from 100 mL to 1 mL, which leads to an increase of the sensitivity. In this way a detection within the statutory provisions of 100 cells/mL is possible.

Heat-inactivated *S. aureus* could be detected at the Immunomat, the old flow system, down to 1.3·104 cells/mL. The first optimizations have been done with heat-inactivated S. aureus at the MCR3, the new microarray flow system with heated flow cell. This new heating element offers new possibilities, for example a reduction of detection time from 60 min down to 15 min.

The next microarray experiments will be done with living *S. aureus* and *B. cereus* spores and then a combination of separation and enrichment will be performed.

S. Ott

Aerosol Research (Prof. R. Niessner)

Characterization of Laboratory-Produced Internally Mixed Iron-Containing Soot Aerosols

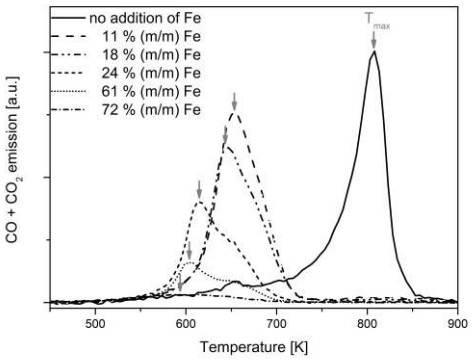
Funding: DFG, RFBR
Cooperation: Institute of Nuclear Physics, Moscow State University

Soot is a major pollutant in the atmosphere of urban areas and often contains not only carbonaceous matter, but also inorganic material, i.e. Fe compounds, originating from impurities in fuel or lubricating oil, fuel additives or engine wear, may change the physico-chemical properties of soot and hence its impact on the environment.

Iron-containing soot was prepared in a propane/air diffusion flame. By adjusting the seed amount of iropentacarbonyl $Fe(CO)_5$ to the flame, soot samples of various Fe content were generated. Scanning Electron Microscopy and Energy-dispersive X-Ray Microanalysis (SEM/EDX) were combined with Cluster Analysis (CA) to investigate single particles of iron containing soot. Comparing relative contents of C, O and Fe measured by SEM/EDX in single particles, CA revealed the presence of different groups of single particles: those particles that only contain C, those that consist of C and O and those that are composed of C, O and Fe.

Furthermore, X-Ray Photoelectron Spectroscopy (XPS) proved that Fe contaminations in the laboratory-produced soot are most dominantly present in the highest oxidation state (III). Raman Microspectroscopy (RM) and Infrared Spectroscopy revealed the graphitic soot structure and were used to characterize present hydrocarbons and iron species. Fe addition did not change the soot structure significantly, but seeding of the flame with $Fe(CO)_5$ led to an increase of the ratio of aliphatic to aromatic hydrocarbons, while the total amount of hydrocarbons decreased with increasing Fe content. Moreover, Fe is most dominantly present as amorphous Fe(III) oxide that crystallizes upon thermal treatment of soot to form hematite.

For analysis of soot reactivity, Temperature-Programmed Oxidation (TPO) was applied. Soot sampled on quartz fiber filters was combusted in a stream of nitrogen (3 L/min) with 5 % of oxygen from 373 K up to 973 K. The temperature T_{max} of maximum emission of CO and CO_2 was used as criterion for soot reactivity. TPO profiles generally showed two emission modes (see figure). The minor emission is assigned to the combustion of nonvolatile hydrocarbons or Fe carbides. Its position hardly shifts with varying Fe content. The major mode can be attributed to the combustion of soot internally mixed with Fe impurities. T_{max} of this mode strongly depends on Fe content, as it follows an exponential decay with increasing Fe content in soot. The ratio CO/CO_2 at T_{max} decreases with increasing Fe content, indicating that Fe (III) oxide promotes complete oxidation of soot.



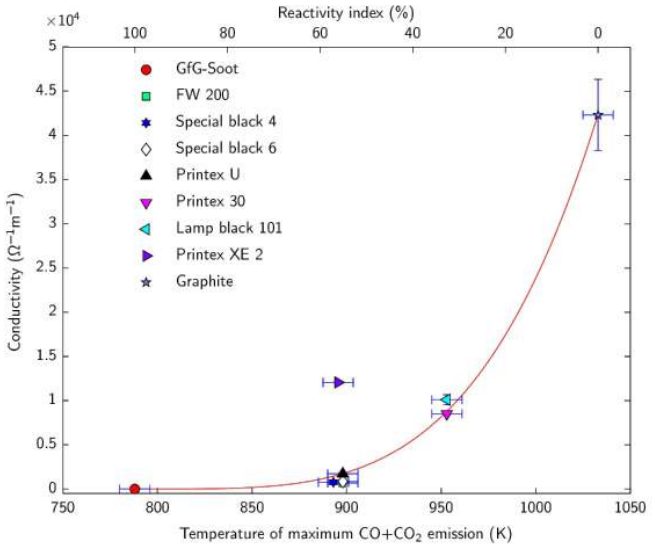
TPO profiles for six propane soot samples of different Fe content normalized to soot mass on filter

H. Bladt, N. P. Ivleva

Conductivity for Soot Sensing: Possibilities and Limitations

Funding: Audi AG, Ingolstadt
Cooperation: Audi AG, I/EA-821

Atmospheric aerosol particles are of great concern to air quality. Current and upcoming regulations for vehicle emissions require the removal of particulate emissions from diesel engines. Currently, ceramic wall-flow diesel particle filters (DPF) have been enforced to reduce the total particle mass and the particle numbers in the exhaust. On-board control is necessary for premature detection of a malfunction of DPF systems. Here, cheap and reliable tools are required to detect and analyze soot particles on-line. Conductometric soot sensors have the advantage of simplicity, low costs and especially small dimension. Their properties make them suitable for on-board monitoring of particular matter emission of diesel engines.



Correlation of soot conductivity and soot reactivity

A car with a Euro VI diesel engine was equipped with conductometric sensors and an AVL Micro Soot Sensor (MSS) as validation device. We developed a thermophoretic precipitator connected with an interdigital electrode sensor to combine the conductivity measurement principle with a controlled and size independent deposition method and to compare two different systems on-line under real live conditions.

Extensive test rides showed the potential of the conductometric approach to accurately detect soot concentrations after a partially bypassed DPF. By including public overland, inner city, uphill and highway scenarios with high velocities the performance of in exhaust gas mounted sensors was assessed. To gain more detailed information we reproduced several conditions on a test track and could shed light on different phenomena. With our external thermophoretic precipitator with an interdigital electrode we could show even better correlations with the MSS reference.

In laboratory experiments the influence of microstructural properties and the impact of inorganic admixtures of carbonaceous materials were investigated. With Raman microspectroscopy and temperature-programmed oxidation with the electrical conductivity of several carbon blacks and soot, it has been shown that the conductivity of carbon materials is strongly influenced by the microstructure. Therefore it was possible to correlate the conductivity directly with the soot oxidation reactivity.

J. Schmid, B. Grob

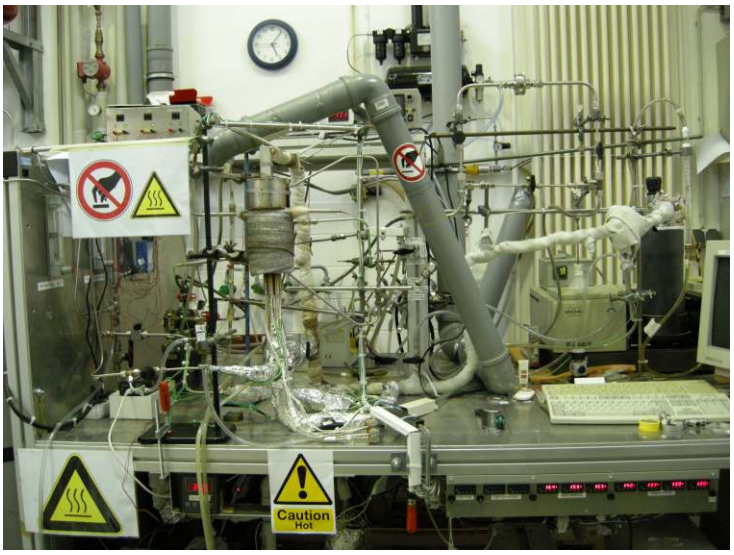
Linking Reactivity and Oxidation Kinetics to Soot Structure

Funding: FVV (Association for Combustion Engine Research)
Cooperation: MAN/SE, Daimler AG

To improve the overall air quality, the reduction of soot nanoparticles emitted by diesel engines is essential. In order to meet the present and future emission limits, soot particles must be filtered from the engine exhaust. Diesel particulate filters, which have been applied for this purpose, need to be regenerated. The efficiency of the regeneration step is strongly affected by the oxidation behaviour of the deposited soot. Highly reactive soot can thereby reduce the energy costs of the regeneration step (due to shorter combustion times and lower temperatures). Due to the higher oxygen content bio fuels can provide additional potential for fostering soot oxidation, while reducing the carbon footprint.

The reactivity and oxidative kinetic studies of soot are done by Temperature Programmed Oxidation (TPO). Therefore the TPO test bench has been modified for temperatures up to 750 °C to allow for full oxidation of different soot samples, while preserving a well defined temperature profile for the kinetic studies. However, TPO experiments are very time and cost consuming. On the other hand, one can also obtain information about the reactivity of soot by measuring the structure with Raman Microspectroscopy (RM). Raman spectra show peaks at 1580 cm^{-1} (G or “Graphite” peak) and 1350 cm^{-1} (D or “Defect” peak). D and G peaks exhibit strongly varying relative intensities and widths for different (bio) diesel soot samples.

We developed Multi-wavelength Raman microspectroscopy (MWRM) analysis for characterization of soot structure and reactivity. This method is based on the dispersive character of carbon D mode in Raman spectra (i.e. red shift and increase in intensity at higher excitation wavelength, $\lambda 0$). The approach has been proven by investigating various diesel soot samples and related carbonaceous materials at different $\lambda 0$. The different TPO experiments characterize the oxidation behaviour and allow us to evaluate the CO and CO2 emission and the mass loss over the temperature. Ongoing experiments show a clear impact of fuel composition on the reactivity. Further studies are focused on investigation of the kinetic aspects at several temperature points for several hours to gain detailed information about the different soot types and the potential impact on DPF regeneration.



Photograph of the experimental setup

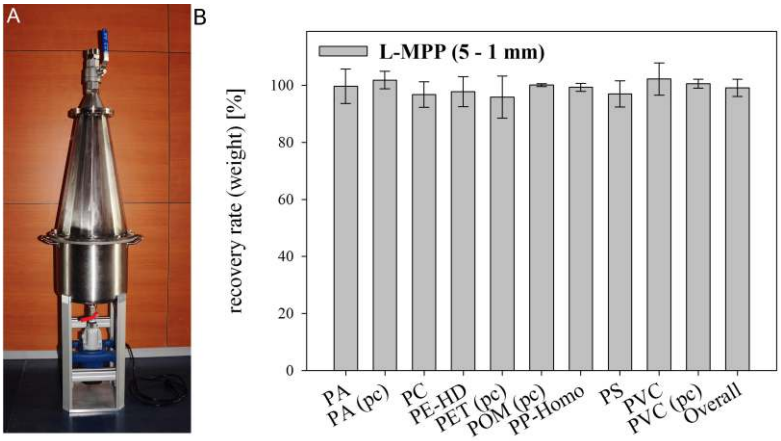
The prediction capabilities of MWRM will be expanded to the structure-reactivity correlation of bio-diesel.

J. Schmid

New Efficient Method for the Quantification of Plastic Particles in Sediments of Aquatic Environment

Funding: DFG
Cooperation: Prof. Dr. Laforsch, LMU, Munich

In recent years the pollution of marine environments with plastic waste has been well documented. High amounts of plastic particles accumulate in the sediments and in the pelagic zone and can be ingested by many organisms.



Experimental setup and recovery rates for the fractionation of plastic particles

Therefore the plastic accumulates in the food chain and poses a risk to humans and the environment. Nevertheless the impact on aquatic ecosystems is not yet fully understood. Moreover, only a few studies are known concerning the amount of discharged plastic particles to freshwater environments. Therefore, there is a high requirement for scientific studies to examine the potential endangerment by plastic particles of these ecosystems.

A first important step in order to study the consequences of plastic debris in aquatic ecosystems is a reliable, verified and standardized method to quantify the amount of plastic particles. We developed an accurate method based on density separation in a $ZnCl_2$ solution (at density 1.6 - 1.7 kg/L), which allows for an extraction and quantification of plastic particles from sediments of aquatic environments. Furthermore, we constructed a Plastic Sediment Separator (PSS) which enables a reliable separation of different types and size classes of plastic particles from sediment samples (see Figure A). Our study is the first providing validated recovery rates of 99.1% for large micro-plastic particles (L-MPP, 1 - 5 mm) and 95.5% for small micro-plastic particles (S-MPP, <1 mm), see Figure B. Moreover, the recovery rate using density separation was significantly higher than separation based on froth flotation (ca. 55% for L-MPP) – the method commonly used in the recycling industry. Subsequent identification of the particles with spatial resolution down to 1 µm is performed by Raman Microspectroscopy.

Thus, our new method can be used for a reliable separation, identification and quantification of plastic fragments ranging from meso-plastic particles (5 - 20 mm) to S-MPP (<1mm) from samples of aquatic sediments and even plankton samples.

J. Schmid, N. P. Ivleva

Modelling of Deposition Mechanisms in EGR Heat Exchangers and Experimental Verification

Funding: FVV (Association for Combustion Engine Research)
Cooperation: Institute for Internal Combustion Engines, TUM

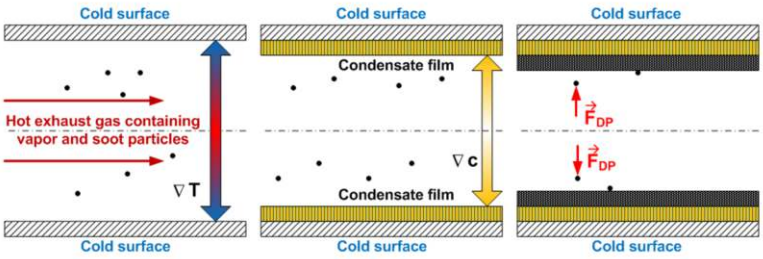
Future emission standards require increased application of exhaust gas recirculation (EGR) which is a very effective way to reduce nitrogen oxide (NO_x) emissions in diesel exhaust gases. Today's EGR coolers are designed to meet the limitations for NO_x output although their efficiency decreases during vehicle lifetime. Therefore EGR coolers are oversized to compensate their rate of fouling by cooling efficiency reserves. Both increased EGR-rates and engine efficiencies are aspects that are more in favor for external rather than internal EGR. An interconnected air-to-water cooler performs the task of reducing the gas temperature in this application.

Besides the usual combustion end products the recycled exhaust gas also contains unburnt hydrocarbons, soot particles metal oxides and traces of sulfuric acid. These incineration residues tend to form insulating deposits on the gas side of the EGR cooler which reduce heat transfer and thus the cooling efficiency of the device.

The work performed during this project was based upon the experimental results from a previous FVV project. The thermophoretic and diffusiophoretic velocities of the soot particles inside the cooler were calculated. The results allowed to draw conclusions on the deposition efficiency of these mechanisms which were validated using experimental data also obtained during the course of the project.

Based on the experimets and modelling results the following recommendations for cooler design and minimization of fouling during cooler operation can be drawn.

To avoid particle deposition by diffusion a tube geometry with a large cross section is needed. High gas velocities are preferable to reduce the residence time of the particles inside the cooler.



Principle of diffusiophoresis

To reduce particle impaction, the cooler geometry has to be free of obstacles and sharp bends. Stagnation of the gas should be avoided, because long residence times can lead to particle growth by accumulation.

Thermophoresis is best reduced by ensuring small temperature gradients within the cooler. Large cross sections and high flow velocities also help in reducing the thermophoretic effect.

Diffusiophoresis within the cooler is one of the most important deposition mechanisms (see figure). It can easily be avoided by choosing conditions, under which no vapor condensation occurs. This is achieved best by keeping wall temperatures at a high level. As some of the recommendations contradict the cooler's purpose, a compromise between avoidance of cooler fouling and cooler efficiency must be found.

G. Hörnig, M. Hager

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T. Baumann, C. Mayr and R. Niessner, Hydrochemisches Monitoring als Werkzeug zur Charakterisierung von Thermalbohrungen, Der Geothermiekongress, 11.-15.11.2011, Bochum.

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R. Niessner, Characterization of Soot - Pitfalls & Possibilities, Austrian Academy of Sciences, 30.06.2011, Vienna, Austria (invited lecture).

R. Niessner, Microarray Technology as Future Tool to Exonerate Classical Analysis, IUPAC International Congress on Analytical Science, 22. - 26.05.2011, Kyoto, Japan (invited lecture).

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R. Niessner, Progress in Microarray-based Analysis EUROanalysis, 11.09. -15.09.2011 Belgrad, Serbia (invited lecture).

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C. Helmbrecht, N. P. Ivleva, R. Niessner, Monodisperse Calcium Carbonate Particles in different Morphologies as Reference for Particle Shape, ANAKON, 20.-23.3.2011, Zürich, Switzerland.

C. Helmbrecht, R. Niessner, Continuous Separation of Hydrocolloids by Photophoresis, ANAKON, 20.-23.3.2011, Zürich, Switzerland.

C. Helmbrecht, R. Niessner, Enrichment of Nanoparticle Suspensions by Directional Freezing of Water, ANAKON, 20.-23.3.2011, Zürich, Switzerland.

C. Helmbrecht, N. P. Ivleva & R. Nießner, Monodisperse Calciumcarbonat-Partikel unterschiedlicher Morphologie als Referenz für Partikelform, ANAKON 2011, 22.-25.03.2011, Zürich, Schweiz.

E. Heuer, K. Späth, R. Niessner and T. Baumann, Cybutryn in einem oberbayerischen Binnengewässer, Wasser 2011, 30.5.-1.6.2011, Norderney.

G. Hörnig and R. Niessner, The role of diffusiophoresis in fouling of exhaust gas recirculation heat exchangers, EAC 2011, 04. - 09.09.2011, Manchester, United Kingdom.

G. Hörnig and R. Niessner, Analysis of Soot Particle Deposition on the Gas Side Surface of Exhaust Gas Recirculation Heat Exchangers, ANAKON 2011, 22.-25.03.2011, Zürich, Switzerland.

S. Huckele, N. P. Ivleva, B. Weinzierl, U. Schumann, R. Nießner, C. Haisch & T. Baumann, Immission von Vulkanpartikeln in die Hydrosphäre, ANAKON 2011, 22.-25.03.2011, Zürich, Switzerland.

S. Huckele, B. Weinzierl, R. Niessner, C. Haisch, T. Baumann & N. P. Ivleva, Identification of Eyjafjallajökull volcanic ash particles collected in Munich in spring 2010 by Raman microspectroscopy European Aerosol Conference, EAC 2011, 4.-9.09.2011, Manchester, UK.

N. P. Ivleva, M. Wagner, H. Horn, R. Nießner & C. Haisch, In situ chemische Charakterisierung von Biofilmen mittels Raman-Mikroskopie (RM) und oberflächenverstärkter Raman-Streuung (SERS) ANAKON 2011, 22.-25.03.2011, Zürich, Switzerland.

N. P. Ivleva, M. Wagner, H. Horn, R. Nießner & C. Haisch, In situ Chemical Imaging der Biofilmmatrix mittels Raman-Mikroskopie und oberflächenverstärkter Raman-Streuung (SERS) Wasser 2011, 30.05.-01.06.2011, Nordeney.

X.Y.Z. Karsunke, R. Niessner and D. Knopp; Entwicklung immunologischer Methoden zur Detektion von Benzo[a]pyren im Trinkwasser. Wasser 2011, 30.05.-01.06.2011, Norderney.

S. Lengger, M. Rieger, L. Pei, R. Niessner, M. Seidel, Fast Enrichment and Quantification of Waterborne Pathogens by qPCR, Medical Biodefense Conference, 25.-28.10.2011, München.

C. Mayr, R. Niessner and T. Baumann, Hydrochemische Charakterisierung einer untypischen Thermalwasserbohrung, Wasser 2011, 30.5.-1.6.2011, Norderney.

C. Mayr, R. Niessner and T. Baumann, Die Isotopen ^{34}S, ^{18}O und ^{2}H als Indikatoren Für die Genese von Tiefenwässern im bayerischen Molassebecken, ANAKON 2011, 22.-25.3.2011, Zürich, Switzerland.

C. Metz, T. Baumann, R. Niessner, B. Ungerböck and T. Mayr, Investigation of pore scale processes at biogeochemical interfaces using micromodels with chemical sensors, ANAKON 2011, 22.-25.3.2011, Zürich, Switzerland.

S. Ott, R. Niessner, M. Seidel: Detection of Microorganisms in Milk after Monolithic Immunofiltration. ANAKON 2011, 22.-25.03.2011, Zürich, Switzerland.

L. Pei, S. Ott, S. Prell, R. Niessner, M. Seidel, Enrichment of Viruses and Bacteria with Monolithic Affinity Columns, ANAKON 2011, 22.-25.03.2011, Zürich, Switzerland.

S. Prell, L. Pei, M. Rieger, R. Niessner, M. Seidel, Fast Quantification of Viruses and Bacteria with a Flow-through Chemiluminescence DNA Microarray in Water, ANAKON, 22.-25.03.2011, Zürich, Switzerland.

S. Prell, R. Niessner, M. Seidel, Development of a Flow-through DNA Microarray for the Detection of Viruses and Bacteria in Water, Wasser 2011, 30.05.-1.06.2011, Norderney.

M. Rieger, L. Pei, R. Niessner, M. Seidel, Combination of Crossflow ultrafiltration and Monolithic Enrichment for the Fast and Efficient Enrichment of Viruses from Large Volumina (30 m^3) of tap water, Wasser 2011, 30.05.-1.06.2011, Norderney.

M. Rieger, R. Niessner and T. Baumann, Visualization and quantification of processes at biogeochemical interfaces with magnetic resonance imaging, ANAKON 2011, 22.-

25.3.2011, Zürich, Switzerland.

M. Seidel, G. Hartmann, V. Langer, R. Niessner, Production, Sampling and Microarray-based Detection of Bioaerosols Containing E. coli and L. pneumophila, EAC 2011, 4.9.9.2011, Manchester, United Kingdom.

J. Schmid, B. Grob, N.P. Ivleva and R. Niessner, Characterization of Soot Structure and Reactivity Based on Raman Microspectroscopy Reactivity, EAC 2011, 04. - 09.09.2011, Manchester, United Kingdom.

J. Schmid, B. Grob, N.P. Ivleva and R. Niessner Characterization of Soot Structure and Reactivity by Multiwavelength Raman Microspectroscopy, ICCPA 2011, 26. - 30.06.2011, Vienna, Austria.

J. Schmid, B. Grob, R. Niessner and N.P. Ivleva, Multiwavelength Raman Microspectroscopy for Rapid Prediction of Soot Reactivity, ANAKON 2011, 22. - 25.03.2011, Zürich, Switzerland.

A. Szkola, K. Campbell, B.G. Dorner, R. Dietrich, E.P. Märtlbauer, R. Niessner, M. Seidel, Microarray Platform for Rapid Quantification of Multiple Biological Warfare Agents, Medical Biodefense Conference, 25.-28.10.2011, München.

A. Szkola, R. Niessner, M. Seidel, Detection of Biotoxins Using Antibody Microarray. ANAKON 2011, 22.-25.03.2011, Zürich, Switzerland

V. Langer, S. Ott, L. Pei, M. Rieger, R. Niessner, M. Seidel, Method for Combining Enrichment and Detection of L. pneumophila in Tap Water, Wasser 2011, 30.05.-1.06.2011, Norderney.

V. Langer, G. Hartmann, R. Niessner, M. Seidel, Detection of L. pneumophila in Bioaerosols Using Antibody Microarrays, ANAKON, 22.-25.03.2011, Zürich, Switzerland.

S. Vazac, R. Niessner and D. Knopp; Hapten Microarray-based Screening of Mycotoxins in Cereals. BIODEFENSE 2011, 25.10.-28.10.2011, München.

S. Vazac, R. Niessner and D. Knopp; Mycotoxin Microarray for Food Analysis. ANAKON, 22.-25.03.2011, Zürich, Switzerland.

K. Wutz, C. Habel, K. Kloth, C. Baumgartner, R. Dietrich, E. Maertlbauer, T. Westermair, F. Braun, P. Walser, R. Niessner, M. Seidel, Validation of a Multianalyte-Immunoassay-Microarray: Analysis of Antibiotics in Raw Milk. ANAKON 2011, 22.-25.03.2011, Zürich, Switzerland.

Hydrochemical consulting

Mineralisation control analyses: Bad Abbach, Bad Aibling, Bad Birnbach, Bad Füssing, Bad Griesbach, Bad Gögging, 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 Wörishofen, Bad Gögging, Sibyllenbad, Erding, Bad Füssing, Bayreuth, Bad Wiessee, Bad Tölz, Fürth

Deep Hydrogeothermal Energy Exploration: Aschheim, Dürrnhaar, Erding, Kirchstockach, Oberhaching, Pullach, Sauerlach

Theses

PhD Theses

MSc Laura-Anne Gérard: High-Resolution Single-Particle Quantification of Colloid Transport Processes.

Dipl.-Chem. Xaver York Zacharias Karsunke: Entwicklung immunanalytischer Methoden zur Detektion von niedermolekularen toxischen Verbindungen in Lebensmitteln.

MSc. Maria Knauer: SERS-Based Label-free Microarray Readout for the Detection of Microorganisms.

MSc. Jimena Celia Sauceda-Friebe: Immunoanalytical Determination of Mycotoxins in Food with an Automatized Instrumental Platform.

Dipl.-Ing. Michael Wagner: Anwendung und Vergleich bildgebender Verfahren zur qualitativen und quantitativen Charakterisierung der Struktur von Biofilmen in der Mikro- und Mesoskala.

M.Sc. Theses

BSc Lim Zhi Cheng: Microbial Fuel Cells for Wastewater Treatment.

BSc Dominik Deyerling: Particle Measurements at an Engine Test Bench of a Heavy Duty Engine.

Cand. phys. Benedikt Grob: Charakterisierung und elektrische Leitfähigkeitsmessung an Aerosolen.

BSc Andreas Huber: Detektion von perfluorierten Tensiden mittels HPLC-MS.

BSc Mark Lafogler: Colloid-associated Phosphorous Transport in Heterogeneous Alluvial Gravel Aquifer Media.

Cand.chem. Kathrin Schwarzmeier: SERS-Based Microarray Readout.

BSc Shen Pei Joanna: Development of New Ion Exchange / Bipolar Membranes for Electrochemical Water Treatment Processes.

Cand. ing. Christian Tyroller: Bewertung von Partikelanzahlmesstechnik.

BSc Sebastian Wohlfahrt: Screening und Charakterisierung neuer, hoch affiner monoklonaler Antikörper gegen Ochratoxin A.

B.Sc. Theses

Nora Abbas (B. Sc. Geol. Wiss.): Hydrogeologische und hydrochemische Untersuchungen an Mineralquellen im Gebiet westlich vom Kloster Teplá in Westböhmen (Tschechien).

Thomas Burmeister: Bestimmung der elektrischen Leitfähigkeit von Kohlenstoffhaltigen Verbindungen.

Christian Fetzer: Optimization of Extraction and Immunological Determination of Fumonisin B1 in Crops.

Kerstin Mayer: Studies of Soot Aerosols by Photoacoustic Sectroscopy and Photophoresis.

Simon Moosmang Conductivity and Reactivity Determinations at Impurity-Containing Carbonaceous Compounds.

Ana-Catherine Neumann: Determination of the Sensitivity and Selectivity of Recombinant Antibody Fragments (scFv) Against Benzo[a]pyrene.

Christina Peinelt (B. Sc. Geol. Wiss.): Hydrogeologische und hydrochemische Untersuchungen an Mineralquellen südöstlich vom Kloster Teplá, Tschechisce Republik.

Maria Reißner: Enrichment and Detection of Viruses in Tap Water by Means of Cross-flow - Ultrafltration and Plaque – Assay.

Klemens Maria Thaler: Photophoresis and Photoacoustic of Aerosols: Chaacterization, Comparsion and Aging.

Jan Vomacka: Develpment of a Flow-Through-Chemiluminescence-Microarray for Detection of Saxitoxin.

Tilo Zollitsch: LED-Induced Fluorescence Spectroscopy.

Institute Colloquia

Prof. Dr. Joachim Wegener, Institut für Analytische Chemie, Chemo-und Biosensorik, Regensburg: Animal Cells Plus Substrate-Integrated Transducers: A Versatile Concept for Whole-Cell Biosensors (21.01.2011)

Prof. Dr. Jeroen Buters, ZAUM – Center for Allergy and Environment, Laboratory for Toxikology and Exposure Research, Technische Universität München: Allergenic Pollen and Allergens in Ambient Air in Europe (18.03.2011)

Prof. Dr. Christian Klampfl, Institut für Analytische Chemie, Johannes Kepler Universität in Linz/Austria: Hyphenation - a Key to Solve Complex Analytical Problems (29.03.2011)

Prof. Dr. Michael Lämmerhofer, Universität Wien, Fakultät für Chemie, Institut für Analytische Chemie: Role of Molecular Recognition and Chromatographic Selectivity in Modern Analytical Methodologies (08.04.2011)

Prof. Dr. F.-M. Matysik, Institut für Analytische Chemie, Universität Regensburg: Chemical Analysis Based on Capillaries or Microchannel Systems in Conjunction with Electrochemical and MS Detection (02.05.2011)

Prof. Dr. J. Christopher Hall, University of Guelph, Canada: Plant Expression of Antibodies Against Her2 Positive Breast Cancer, Biological Weapons, and Environmental Contaminants (06.06.2011)

Dr. Axel Rosenhahn, Institut of Technology Karlsruhe, Institut of Functional Interfaces: Model Surfaces, Microfluidics and Holography for a Mechanistic Understanding of Biofouling (19.09.2011)

Prof. Dr. Matthias Zessner, Vienna University of Technology, Institute for Water Quality: Foam in the Aquatic Environment - Reason for Public Concern (23.09.2011)

Dr. Ann-Kathrin Kniggendorf, Gottfried Wilhelm Leibniz Universität Hanover: Confocal (Resonance) Raman Micro-Spectroscopy as a Tool for Biofilm Analysis (10.10.2011)

Dr. habil. Axel Warsinke, Universität Potsdam: Protein Chips- Reality and Vision (14.10.2011)

Prof. Dr. Oliver J. Schmitz, University of Wuppertal, Institute for Pure and Applied Mass Spectrometry: Atmospheric-Pressure Laser Ionization (APLI) in Trace Analysis: Scientific Findings , Latest Developments and Outlook (03.11.2011)

Prof. Dr. Walter Vetter, Universität Hohenheim, Institut für Lebensmittelchemie: Polyhalogenated Natural Products in the Marine Environment and Food – Identification, Quantification and Evaluation (15.12.2011)

Dr. Derek Persoh, Universität Bayreuth, Lehrstuhl für Pflanzensystematik: Advances in Analysing Mycodiversity in Environmental Samples (16.12.2011)

Teaching

Chemistry (B.Sc. and M. Sc.)

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

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

Chemical Engineering (Diplom)

Aerosol Characterisation (Aerosolcharakterisierung); Niessner

Environmental Measurement Technologies Lab (Praktikum Umweltmesstechik); Niessner, Haisch

Gas Measurement Technologies/Chemical Sensors (Gasmesstechnik/Chemische Sensoren); Niessner

Geosciences (B.Sc. and 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, Hydrochemical and Environmental Analysis Seminar (Hydrogeologisches, Hydrochemisches und Umweltanalytisches Seminar); Baumann, Niessner

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

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. and M.Sc.)

Biochemical Analysis (Biochemische Analytik); Görg, Gierl, Knopp, Nitz, Parlar, Schwab, Seidel
Analytical Chemistry - Separation Techniques, Chemical and Biochemical Sensors (Analytische Chemie - Trenntechniken, chemische und biochemische Sensoren); Knopp
Bioanalytics I: Immunological Procedures; Sensor Technologies (Bioanalytik I: Immunologische Verfahren; Sensortechniken); Knopp
Biochemical and Molecular Biological Methods for Environmental Analysis (Biochemische und molekularbiologische Verfahren in der Umweltanalytik); Knopp
Biochemical and Molecular Biological Procedures for Envrionmental Analysis II - Enzymatic Methods, DNA Probes (Biochemische und molekularbiologische Verfahren in der Umweltanalytik II - enzymatische Verfahren, 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

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

Aerosol Research
1 Aerosol chamber (1 m3)
1 Aerosol flow tube (10 L)
1 Ozone analyzer (UV absorption)
1 NO/NO_2 analyser (Chemiluminescence)
2 Aerodynamic particle sizers (0.5-25 µm)
1 Berner impactor (9 stages, 50 nm - 16 µm)
1 Electrical low-pressure impactor (12 stages, 30 nm - 10 µm)
2 Low-Volume filter samplers (PM 10, PM2.5)
1 High-Volume filter sampler (PM 2.5)
2 Differential mobility particle sizer systems (10-1000 nm)
2 Diffusion batteries (5-300 nm)
5 Condensation nucleus counters
3 Electrostatic classifiers (10-1000 nm)
2 Spark-discharge soot aerosol generators (polydisperse ultrafine carbon aerosol)
1 Berglund-Liu aerosol generator (monodisperse aerosols, 0.8-50 µm)
1 Floating bed aerosol generator (powder dispersion)
1 Rotating brush aerosol generator (powder dispersion)

Bioseparation
Crossflow Filter (Inge AG)
Crossflow Filter (Spectrum Laboratories, Inc)
Pressure and Flowrate controlled Crossflow Filtration System (IWC)

Molecular Biology
1 Biacore X100, General Electric
1 Real-time PCR (Light Cycler 480, Roche)

Microarray Technology
3 Chemiluminescence Microarray Reader (PASA, IWC)
3 Chemiluminescence Microarray Reader (MCR 3, IWC)
1 Ink-Jet Microdispenser (Nanoplotter, GeSim)
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)
1 Clean bench (Herasafe KS, Kendro)
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 (Memmert HCP 108)
2 Fluorescence reader systems, time-resolving
3 Photometric reader systems
1 384-channel washer, Biotek
1 Turbidometer (WTW GmbH)
1 Nanophotometer (Implen GmbH)

Chromatography and Particle Separation
3 GCs with FID, NPD, ECD, TEA, and AED
1 Orbitrap-based benchtop MS, Exactive/HCD-System, Thermo Fischer
1 High-resolution GC/MS, VG Autospec

1 GC/MS for Gas analysis, Shimadzu
1 Portable Micro-GC, MITEC
1 Asymmetrical Field-flow-fractionation system
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 LC system, ECONO
1 Preparative HPLC
1 Zetaphoremeter, SEPHY

Elemental Analysis

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

Laser

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

Optoelectronics/Spectrometer

1 Rowland spectrometer
2 Echelle spectrometer
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 Boxcar integrator
4 Digital storage oscilloscopes (400 MHz, 500 MHz)
3 Optical multichannel analysators with monochromators, time-resolving
3 Intensified CCD cameras
1 Wavemeter

SEM/Microscopy/Raman-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 Laser Raman microscope, Renishaw (514/633/780 nm)
1 Laser Raman microscope, Horiba LabRam (532/633/785 nm)

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 2011

Permanent Staff

Univ.-Prof. Dr. Reinhard Niessner
PD Dr. Thomas Baumann
Univ.-Prof. Dr. Christoph Haisch
Dr. Clemens Helmbrecht
Dr. Natalia P. Ivleva
apl. Prof. Dr. Dietmar Knopp
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

Dipl.-Chem. Henrike Bladt
Dipl.-Phys. Benedikt Grob (4/11-)
Dipl.-Ing. Moritz Herbrich (6/11-)
Dipl.-Ing. Gabriele Hörnig
Dipl.-Ing. Susanne Huckele (-7/11)
Dipl.-Chem. Xaver Karsunke (-7/11)
MSc Chem. Maria Knauer (-7/11)
MSc Chem. Veronika Langer
MSc Chem. Sandra Lengger
Dipl.-Chem. XiangJiang Liu
Dipl.-Geol. Christina Mayr (-6/11)
MSc Chem. Christian Metz
Dipl.-Ing. Andrea Okroy (-4/11)
MSc Chem. Susanna Oswald
MSc Chem. Sonja Ott
MSc Pharm. Anal. Lu Pei
MSc Chem. Michael Pschenitza (4/11-)
MSc Chem. Martin Rieger
MSc Ing.Hydrogeol. Sabine Sailer (-9/11)
Dipl.-Chem. Kathrin Schwarzmeier (7/11-)
Dipl.-Chem. Johannes Schmid
MSc Chem. Agathe Szkola
MSc Chem. Jan-Christoph Wolf
MSc Chem. Klaus Wutz
MSc Chem. Haibo Zhou (11/11-)

External PhD Students

Dipl.-Phys. Peter Menzenbach (INNOLAS, Krailling)
Dipl.-Ing. Michael Wagner (LS Siedl.-Wasserw., -12/11)
Dipl.-Ing. Daniel Müller (ABF München, 7/11-)
Dipl.-Biol. Carmen Kocot (Institut Klinische Pathobiochemie München, 4/11-)

Diploma Students/MSc Students

Christoph Berger (6/11-5/12)
BSc Chem. Sabine Dvorski (4/11-9/11)
Cand. phys. Benedikt Grob (4/10-3/11)
Markus Hager (12/11-5/12)
BSc Chem. Andreas Huber (3/11-9/11)
BSc Chem. Kathrin Schwarzmeier (12/10-5/11)
BSc Chem. Sebastian Wohlfahrt (5/11-10/11)

External Diploma Students

Ruili Feng (BASF, GIST Singapore, 9/11- 3/12)
Zhi Cheng Lim (GIST Singapore, 9/10-2/11)
Dominik Deyerling (MAN Nürnberg, 4/11-10/11)
Meera Mahle (BASF, 9/11-3/12)
Pei Joanna Shen (GIST Singapore, 9/10-2/11)
Cand. Ing. Christian Tyroller (MAN Nbg., 10/10-3/11)

Guests and Research Fellows

Li Dongyang (Uni Zhejiang China,1/11-6/11)
Norriyuki Fujii (Uni Kyushu Japan, 1/11-3/11)
Prof. Dr. Irena Goryacheva (Uni Saratov Russia, 1/11)
Elena Kireeva (Uni Moscow, 9/11-12/11)
Prof. Dr. Popovicheva (Uni Moscow, 2/11-3/11, 9/11)
Elena Speranskaya (Uni Saratov Russia, 10/11-3/12)
Ilya Voronov (Uni Saratov Russia, 10/11-3/12)

Student Assistants

Beatriz Mor Fernandez (10/10-3/11)
Sebastian Weiker (12/09-5/11)
Sebastian Wohlfahrt (8/10-1/11)