Technische Universität München

Annual Report 2012

Institute of Hydrochemistry and Chemical Balneology
Chair for Analytical Chemistry

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Chair for Analytical Chemistry
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Editor: Dr. Thomas Baumann

Editorial

Dear coworkers, friends & colleagues!
It is my great pleasure to present you the annual report for 2012, a year which ce can safely consider successful and very satisfying.

Our plans for the new Munich Center for Water Research have been submitted and are just now waiting for financial and scientific approval. This interdisciplinary center will integrate several water related disciplines and will be situated in a new building on the Garching campus of TUM. We are also happy that the IWC will be strongly represented within this concept, which confirms our long-term strategy to invesitgate processes along the water cycle, from atmosphere to deep geothermal energy.

For many years, the IWC infrastructure provides and fosters interdisciplinarity. For example the aerosol and microarray groups have been working together on the detection of *Legionella spp.* in aerosols from showers and cooling towers. A combination of bioaerosol sampling and fast detection with a chip based immunoassay will provide the necessary tool to fulfill current EU and federal legislation. The development of labeled antibodies against benzo[a]pyrene and their application to visualize the spatial distribution of this contaminant in porous media using magnetic resonance imaging brought together Immunological methods and hydrogeology,

Our Raman lab, headed by Dr. Ivleva, is another "hot spot" at the institute connecting young researchers from different fields. Looking at the uptake of plastic garbage from lake sediments by daphnia, as in a new DFG project together with limnologists, and the assessment of the impact of nanoparticles on aquatic systems, including daphnia, as in a DFG research unit in the hydrogeology group, seem not too far apart in terms of the measurement techniques and can greatly benefit from each other, given an infrastructure like the IWC. You will find further examples underlining the importance of interdisciplinar research in this annual report and on our web pages.

Interdisciplinar research, however, requires larger structures. The concept of micro research units, although very flexible at first glance, has a tendency to lead to highly individual, sometimes encapsulated groups with little interaction unless embedded in an institute like the IWC or the Munich Center for Water Research. This is why all of us are wholeheartedly supporting this initiative.

Quite a number the long-term developments we presented in recent years are now commercially available. Some in routine analysis, like the photo-acoustic soot sensor, some in dedicated laboratories, like the MCR3, and some in research applications, as our multi-step filtration and separation unit for viruses and microorganisms, MMC3. But not only measurement devices are on the market, our anti-benzo[a]pyrene antibody is still evaluated to fly to Mars with the next ESA EXO Mars mission. Likewise our hydrochemical models are find their application deeply underground as a tool to predict and optimize the performance of geothermal facilities, which has become even more important due to a change of the funding of renewable energy sources.

Finally, I would like to take the opportunity to congratulate Dr. Haisch to the Bunsen-Kirchhoff Award for Analytical Chemistry. It is quite obvious, that this and all other projects would not be possible without your continuous help, financial support, and critical remarks.

Thank you very much and take care,

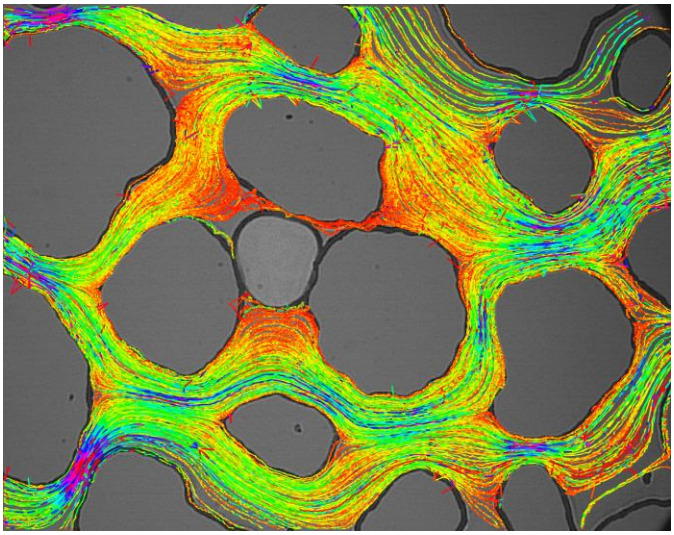
Reinhard Niessner

Hydrogeology (PD Dr. T. Baumann)

Investigating Biogeochemical Interfaces in Soil Using Sensor Micromodels and Raman Microscopy

Funding: DFG (Deutsche Forschungsgemeinschaft)
Cooperation: Partners in the DFG Priority Programme SPP 1315

Biogeochemical Interfaces (BGI) control the fate of organic chemicals and the functioning of the soil as a filter. BGI are formed by microorganisms and are necessary to ensure their survival. Since the pore space in soil is vast from the perspective of a microorganism, it is crucial to a microorganism to use accessible nutrients most effectively. Spatial access to nutrients limits the degradation capability of the soil and the development of BGI's equally.



Color coded trajectories (red = slow, purple = fast) around a gas bubble in a heterogeneous micromodel

Chemical gradients are one of the main driving forces for the transport of contaminants in soil at low Peclet numbers. Here, pore scale resolution of chemical gradients is required to quantify the filter functions in a spatially restricted system. In order to gain access to the pore space a simplified, well controlled 2D pore network etched into silicon wafers is used together with spectroscopic methods. Fluorescence and Raman spectroscopy offer access to the localized concentration of selected contaminants while particle tracking using fluorescent latex beads gives access to the local flow velocities. The latter are of prior importance to assess the mass transfer rates, especially if the whole pore structure cannot be mapped due to technical and temporal limitations. This data together with the pore topology and micro-CT images serves as input data for the flow model of the micromodel.

Silver nanoparticles are used to quantify degradation products of phenanthrene. In contrast to conventional applications of surface enhanced Raman scattering, experiments in microfluidic systems require highly stable nanoparticle aggregates due to a longer time scale of the experiment. With the current preparation procedure, intraday and interday variance are sufficient for experiments up to 96 hours. The dynamic range of the quantification with SERS is 2.5 orders of magnitude, which seems to be sufficient to map gradients at biogeochemical hotspots.

Microbial activity is also accessible through the development of a gas phase in the pore structure. Experimental results indicate, that the bacterial density in the pore throats is smaller than in the pore bodies which makes sense because of the different flow velocities (see Figure).

C. Metz

Minimizing Risks for Geothermal Power Plants

Funding: BMU (Federal Ministry for the Environment, Nature Conservation and Nuclear Safety)
Cooperation: SWM Services GmbH, Munich

The Bavarian Molasse Basin is one of the primary targets for the exploration of deep geothermal energy. South and South-east of Munich, the Malm aquifer dips to more than 3500 m below ground surface and provides thermal water with temperatures of more than 135 °C and a productivity exceeding 100 L/s. While the conditions for effective conversion of geothermal energy to electrical power are favorable, a number of constraints have to be met: gas loading, particle precipitation, and corrosion issues are addressed in this project.

Impressions from the pumping test

At our reference site, the gas loading has been decreasing from up to 500 NmL/L in 2005 to 90 ± 10 NmL/L. Together with this decrease the short term fluctuations decreased significantly. The relative gas composition with methane dominating followed by carbon dioxide and nitrogen is almost constant indicating equilibrium conditions.

The gas composition in the casing of a production well was monitored during the initial pumping tests. The casing was pressurized with nitrogen to avoid a collapse when lowering the water table. The relative concentration of nitrogen was then found to decrease while the relative concentration of aliphatic hydrocarbons increased. It is remarkable, that propane, butane and other hydrocarbons were detected while the concentration of methane was below the limit of detection. This finding can be explained with the development of an oil film along the casing wall as the water table is dropping. Dissolved gases in this oil film will slowly equilibrate with the gas phase in the casing. The equilibrium with the thermal water in the well, in contrast, is limited by the rather small surface area of the water table.

Right after the start of the pump, there we collected a high number of particles containing iron and zinc which is attributed to the mobilisation of corrosion products from the inner casing. Mineral particles include Mg-rich calcite which is precipitating during production due to degassing of carbon dioxide. Later on, particles originating from the aquifer, e.g. dolomite, dominate. Interestingly, metal particles which were rich in copper were detected indicating a failure of the pump which occurred shortly afterwards. As the oil which is produced with the thermal water is significantly changing the filtration efficiency and cutoff values of the filters, there might be a need to redesign the filtration system.

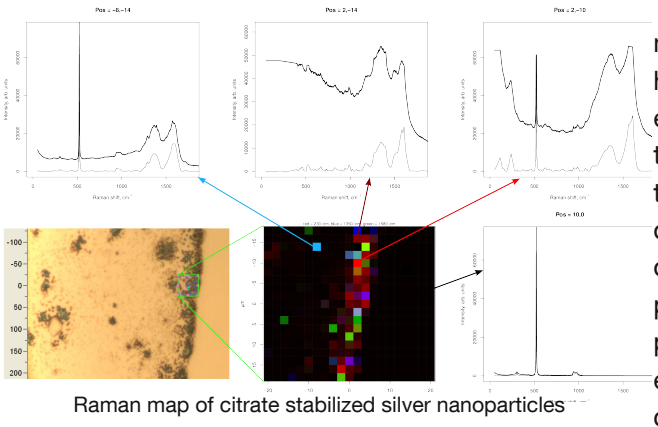
M. Herbrich

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

Funding: DFG (Deutsche Forschungsgemeinschaft)
Cooperation: DFG Research Unit InterNANO (FOR1536)

Diverse applications for engineered inorganic nanoparticles (EINP) lead to an increased emission of nanoparticles into the environment. Once introduced into the environment, EINP are expected to pass the wastewater-river-topsoil-groundwater pathway. In spite of this assumption, only little is known about the processes governing EINP aging and functioning in the environment. The objective of the DFG research unit InterNano is to identify the processes of aging and transfer of EINP at the aquatic-terrestrial interface. We assume aging in the aquatic and terrestrial environment, involves changes of the EINP surface (masking) as well as changes in EINP bulk composition (weathering). Aging processes will affect the mobility of EINP and their interactions with pollutants. Our project aims to identify the processes controlling the transport of EINP in porous media on the microscale. Micromodel experiments will be performed to identify and quantify the effect of local physical heterogeneities on the transport of fresh, weathered and masked EINP.

Changes of the surface properties of EINP during transport are accessible through Raman Microspectroscopy (RM). Experiments are run with TiO_2 and Ag nanoparticles, because these nanoparticles are weakly or not bound in consumer products (e.g. fabrics, sunscreen or paint) and therefore can easily be introduced in the environment. While TiO_2 nanoparticles do show a distinct Raman spectrum and can be measured directly, Ag nanoparticles have to be detected indirectly with RM using the SERS effect. With SERS it is also possible to detect surface coatings on silver nanoparticles.



Raman map of citrate stabilized silver nanoparticles

Natural organic matter is known to have a stabilising effect on nanoparticles. To investigate the influence of organic matter on the transport properties of nanoparticles, first experiments with citrate stabilised Ag nanoparticles and polygalacturonic acid were performed. A solution of citrate stabilised Ag nanoparticles was mixed with polygalacturonic acid and filtered (0.01-µm polycarbonate filter) to separate the coated nanoparticles from dissolved polygalacturonic acid. The filters were sonicated in milliQ-water for 15 minutes to detach the nanoparticles. This washing and filtration procedure was repeated three times. Raman spectra of the nanoparticles were acquired in solution. First results indicate the formation of a stabilising layer of polygalacturonic acid around the nanoparticles.

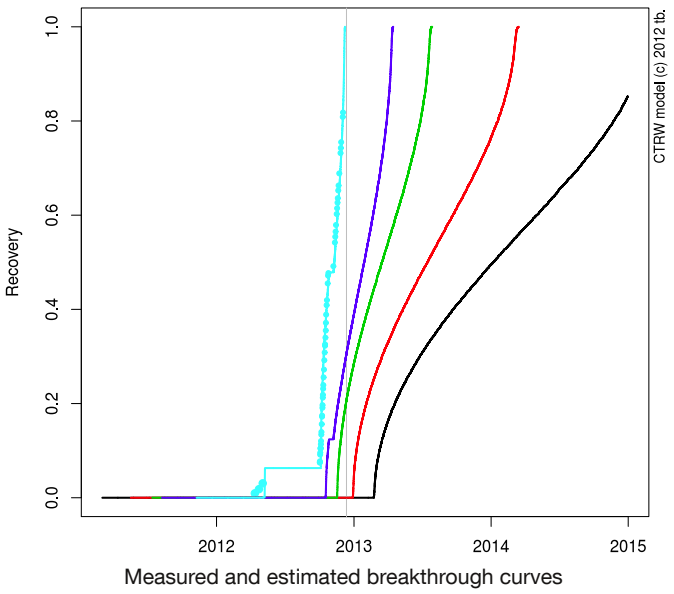
M. Kühn

A Push-Pull Tracer Test at a Geothermal Well

Funding: BMU (Federal Ministry for the Environment, Nature Conservation and Nuclear Safety)
Cooperation: IEP GmbH, Pullach; Erdwerk GmbH, Munich; Aquasoil GmbH, Berlin

Geothermal exploration of the Malm aquifer in Bavaria is highly successful. Data about the long-term operation, however, is still scarce, although detailed knowledge about the processes occurring in the aquifer is a key requirement to run geothermal facilities efficiently and economically.

Usually, there is a constant flow of data from the production well (temperatures, hydraulic data, hydrochemical conditions, gas composition), but not even the temperatures in the immediate surrounding of the reinjection well are accessible or known.



Measured and estimated breakthrough curves

In 2011 the geothermal facility in Pullach was extended with a third geothermal well reaching into the Malm aquifer which is now used as a reinjection well. The former reinjection well was converted to a production well after 5 years of operation. This setting offers a unique opportunity to study the processes in the vicinity of a reinjection well.

The viscosity of the reinjected cold water is 60% higher compared to the production well, therefore an increase of the reinjection pressure as the cold water plume increases around the reinjection well is expected.

Measurements, however, show a significant decrease of the reinjection pressure, suggesting processes in the aquifer which positively change the hydraulic properties and overcompensate viscosity effects. Hydrochemical data and modeling indicate that dissolution of the matrix along the flow pathways is responsible for the decreasing reinjection pressures.

The change of the flow direction in the from reinjection to production was used to conduct a push-pull tracer test. Here, a series of fluorescent dye pulses has been added to the reinjected water before the former reinjection well was shut down (push phase). These tracers included conservative tracers, surface-sensitive tracers, and NAPL-sensitive tracers. After changing to production the tracers will be produced and analysed (pull-phase). Their different behavior within the reservoir will deliver data about dispersion, sorption properties, matrix interaction and the regional flux.

The first tracer breakthrough (see Figure) points to a hydraulic setting with a significant heterogeneity of the flow pathways and that regional flow is not negligible.

M. Lafogler

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

Hapten Microarray-based Screening of Mycotoxins in Cereals

Funding: AiF-FEI (German Federation of Industrial Research Associations), Verband Deutscher Mühlen
Cooperation: Lehrstuhl für Hygiene und Technologie der Milch, LMU München

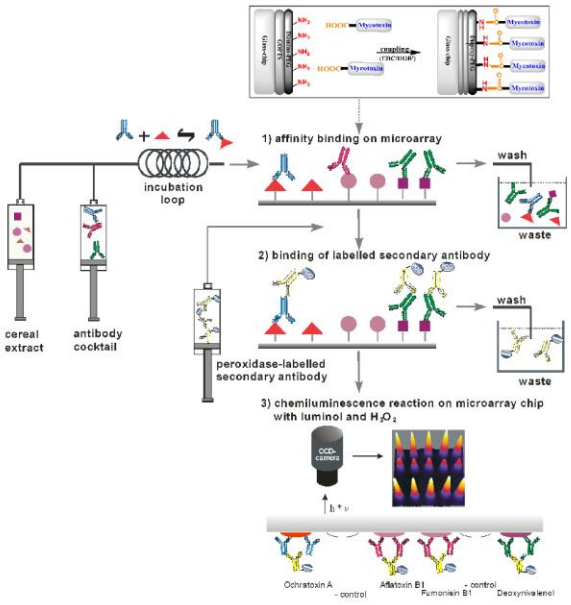
Mycotoxins are a very heterogeneous group of secondary metabolites from fungal species growing on agricultural commodities in the field or during storage. Since they represent a potential health hazard to humans and animals, maximum levels for several mycotoxins in food have been set by the European Commission.

Screening methods for rapid and sensitive detection based on cost-effective and easy to use methods, are dominated by immunochemical tests using anti-mycotoxin antibodies in a variety of different assay formats, but do not allow multiple analyte testing.

The biosensor development, in contrast, focuses on parallel analysis of several mycotoxins. Here, we present an indirect competitive immunoassay on regenerable, reusable glass microchips for the parallel determination of currently four mycotoxins, (aflatoxins, OTA, DON, and FB1), in cereal extracts on a fully automated flow-through device with chemiluminescence readout.

Mycotoxin derivatives are synthesized and then immobilized on PEGylated glass chips yielding a hapten-microarray with a significantly reduced number of steps for chip functionalisation, leading to cost and time savings. Immunological determination takes place in a flow chamber and the chemiluminescence readout is performed by a CCD camera. The microarray chip is reusable up to 40 times. To avoid unacceptable batch-to-batch variation, fabrication of microarray chips should be performed in clean-rooms with controlled environment. The obtained mycotoxin calibration curves show an LOD which meets the regulation limits. The recovery rates of different fortified cereal samples were determined. Furthermore, crude extracts could be measured directly after simple filtration and dilution steps. Further improvement of the extraction yield of some mycotoxins might be expected by fine-tuning of the extractant mixture. The results of an inter-laboratory comparision of wheat samples naturally contaminated with mycotoxins using different analytical methods revealed acceptable agreement.

S. Oswald

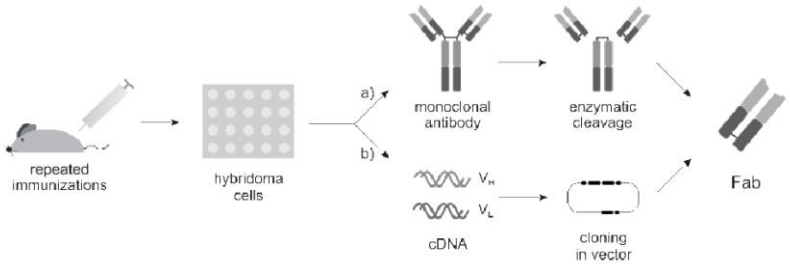


Schematic of mycotoxins bound covalently to the microarray chip

Paratope-epitope Interactions of Monoclonal Benzo[a]pyrene Antibodies and Determination of B[a]P in Edible Oils

Funding: Hanns-Seidel-Stiftung, IWC
Cooperation: Lehrstuhl für Biochemie, TU München, Prof. Dr. M. Groll; Lehrstuhl für Biologische Chemie, TU München, Prof. Dr. A. Skerra; Oil Crops Research Institute, Chinese Academy of Sciences, Wuhan, China, Prof. Dr. Peiwu Li, Dr. Ran Li

Polycyclic aromatic hydrocarbons (PAHs) are formed during incomplete combustion of organic compounds. Because of their high toxicity, limit values were set by the European Commission for benzo[a]pyrene (B[a]P) of 10 ng/L in tap water and 2 µg/kg in edible oils. Sensitive and reliable analytical methods are needed to detect B[a]P at these low concentration.



Enzymatic (a) and recombinant (b) production of Fab fragments

Through optimization of our best antibody (clone 22F12) using a 3-fluoranthenyl-BSA coating conjugate and a poly-HRP labeled secondary antibody, LODs could be lowered 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 in tap water. Recombinant antibodies (scFv) were produced based on the genetic information of three highly affine monoclonal antibodies, but with the scFvs produced yet no further improvement in assay sensitivity could be obtained. As higher sensitivity may be achieved by a genetic manipulation of the antigen binding site, detailed information about the antigen binding site could be gained using X-ray crystallography. For that purpose, Fab fragments of monoclonal antibody 22F12 have to be produced either by enzymatic digestion or recombinant. Crystallization has to be optimized for the B[a]P-antibody complex in order to obtain crystals suitable for X-ray crystallography.

With the existing highly affine monoclonal antibodies an immunological method for the determination of B[a]P in edible oils should be established. To reach this goal, matrix effects have to be minimized, e.g., by effective solid phase extraction of B[a]P to guarantee maximum affinity of the antibodies and thus high sensitivity of the immunoassay. Conventional SPE phases were tested and LODs at the decision level in China (10 µg/kg) could be obtained for olive and sunflower oil samples using silica material as solid phase, however, the selectivity should be optimized further. Possibly, this can be reached by preparation of molecularly imprinted polymers or sol-gel glass immunoaffinity supports and optimization of extraction procedures from these materials. In addition, the fabrication of robust and sensitive lateral-flow tests is under consideration.

M. Pschenitza

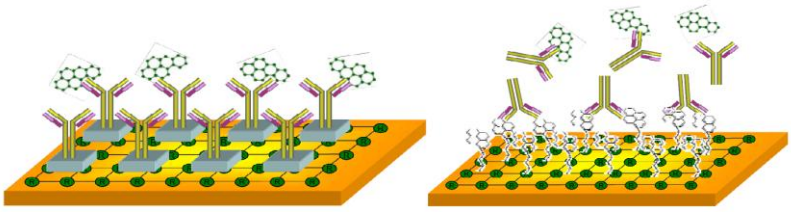
Nanoscaled Architectures for Highly Sensitive Biosensing of Small Molecules

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

The new EU water directive defines the need for a regular monitoring of priority substances and emerging pollutants down to low ng/L, a task which is usually acchieved using costly and time consuming equipment and sample preparation techniques. For efficient monitoring, selective and sensitive high-throughput analyses are required.

The latter requirements are inherent features of immunoassay or biosensors. Many efforts have been made to improve the sensitivity of these immunosensors, a particularly challenging task for low molecular weight contaminants. In general the sensitivity of immunosensors can be increased by improving the quality of the biological material, namely increasing the avidity/affinity of antibodies dedicated to chosen targets, the optimization of their immobilization on the transducer surface, and through amplification of the signal measured by the transduction techniques to be used.

Taking advantage of the complementarity expertises of the three international teams involved, the different routes will be explored aiming at developing a new generation of ultra-sensitive and specific immunosensors. While obtaining the best antibodies relies on modern biotechnological methods, a nanotechnology-based approach will be chosen by the French partners reach the objectives mentioned above. First, transducer surfaces will be nanostructured by functionalizing them in original ways, Second, knowing the remarkable properties of gold nanoparticles for improving analytical performances of several detection techniques, a new alternative strategy will be developed. Better antibody orientation and accessibility, as well as improved sensitivity, are expected from nanohybrid sensing layers. The last part of the project, and also its main objective, will be the detection of targets with high environmental relevance (benzo[a]pyrene, diclofenac, and microcystins) on the novel platforms. This will be achieved by techniques from which indeed an increase of sensitivity and reproducibility is expected on nanostructured surfaces, mainly Quartz Crystal Microbalance with dissipation measurements and Surface Plasmon Resonance. The performance of these “surface” techniques will be systematically compared to results obtained by a newly developed biomolecular multiplexed technique (microarray-based flow-through chemiluminescence ELISA) and LC-MS.



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

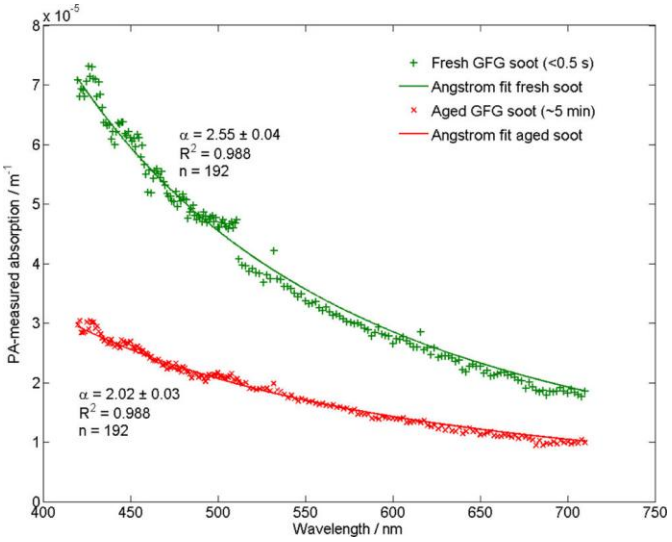
M. Hübner

Applied Laser Spectroscopy (PD Dr. C. Haisch)

Photoacoustic Spectroscopy for Aerosol Analysis

Funding: IWC
Cooperation: Innolas GmbH, GWU-Lasertechnik GmbH, ACAL technology, LIOP-TEC GmbH, Fine Adjustment

Depending on their specific properties, aerosol can be directly hazardous to human health, and influence the global climate. Either directly or as condensation nuclei the Earth's radiation balance can be influenced.



Typical absorption spectrum of soot measured with the PA absorption spectrometer

Hence, monitoring of aerosol particles, and particularly of their optical properties, is crucial. Photoacoustic (PA) spectroscopy is well suitable for this task. The PA effect is based on the optical absorption of electromagnetic radiation, which leads to local heating and expansion. Monitoring of this expansion by a microphone directly reveals the optical absorption, while this PA signal is insensitive to light scattering. Two different photoacoustic systems for aerosol analysis are currently developed and tested, one of exhaust gas analysis and one primarily intended for atmospheric monitoring. The TwinPAS is a new system which allows for the simultaneous, time-resolved analysis of soot and NO_2 in exhaust gas. Beyond the optimization of the analytical figures of merit a focus was set on the practical applicability of the system for routine use in engine testing. Mechanical stability and usability are as important as response time and the possibility to heat the complete gas system to 80 °C. The other system is a PA spectrometer developed for the optical characterization of aerosol particles. Instead of the modulated laser source commonly employed for gas-phase PA, a pulsed wavelength-tunable laser is employed. It gives access to the full spectral range from 410 to 2100 nm. To our knowledge, it is the first tool which allows recording a real absorption spectrum of aerosol particles over the complete UV, visible, and NIR spectrum. Up to now, either aerosol extinction, i.e. absorption plus scattering, is measured, or the analysis is limited to few selected wavelengths and measurements on filter surfaces. The sensitivity of the system in the visible range is in the range of 1 Mm^{-1}.

C. Haisch, P. Menzenbach

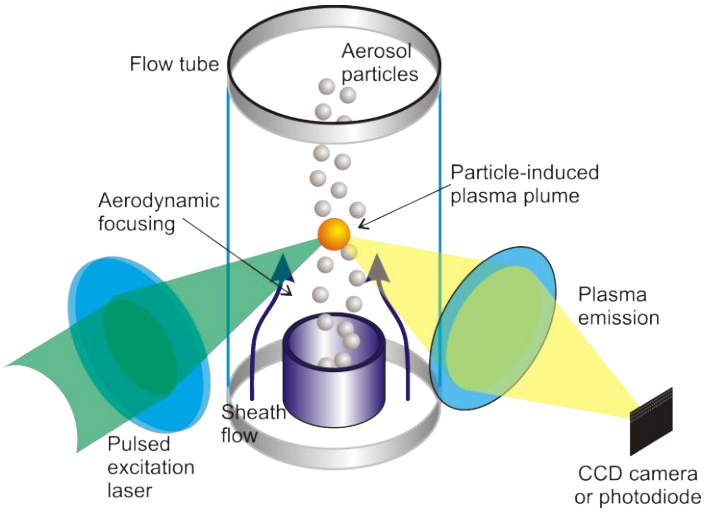
Optical Aerosol Particle Counter

Funding: IWC

Aerosol particles like fine dust are a big problem in our time. Especially soot, which is generated by incomplete combustion e.g. in diesel engines, heating installations, and power plants should be controlled by inducing limiting values. A challenge for analytical chemistry is the development of methods to measure the concentration of aerosol particles and to characterize them. Due to the goal of reducing the output of fine dust and soot, sensitive methods have to be developed that are able to measure small concentrations or better to count single particles. The established techniques for counting different kinds of aerosol particles are Condensation Nucleus Counter (CNC) which are based on the principle of growing particles due to condensation and optical particle counter based on light scattering. An approach already described in literature for counting particles in aquatic solutions is Laser Induced Breakdown Detection (LIBD). The presence of particles reduces the threshold of a plasma breakdown in the field of a pulsed and focused light beam. We use this method for the first time to detect and count aerosol particles. Beyond the particle number density, we hope that the technique also gives access to the particle size and/or optical properties.

For the experiments, soot is generated by a spark discharge generator and diluted with air. In the measuring chamber, the pulsed laser, featuring a pulse repetition rate of 10 Hz, is focused into the sample flow. The luminescent sparks generated by the plasma breakdown induced by particles in the focus are monitored by means of a photodiode. The number particle concentration can be determined by the breakdown probability. An aerosol electrometer is used as a reference for the particle concentration. The energy of the laser pulses is monitored by an energy meter for normalization.

M. Eß



Schematic of the experimental setup

Photofragmentation for the Detection of NitroPAHs in Atmosphere and Exhaust Gas

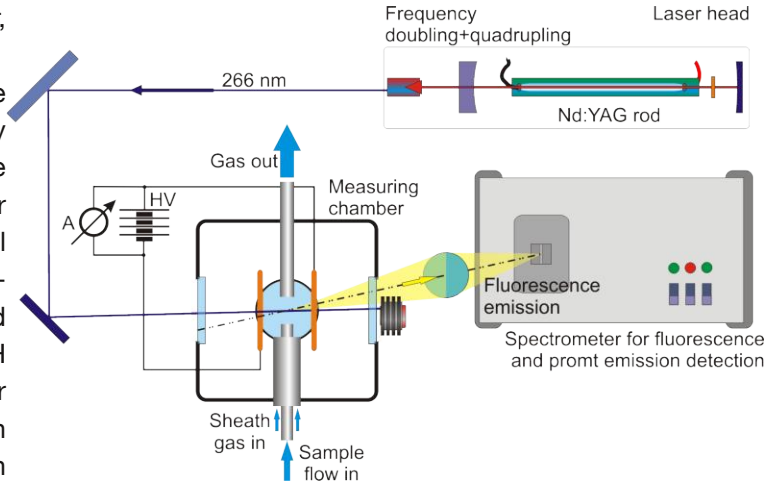
Funding: IWC

Polycyclic aromatic hydrocarbons (PAHs) together with their products formed in air, nitro-PAHs (NPAHs) are probably the abiotic class of substances which is most harmful for human health. This does not only apply for the atmosphere, but the total environment. A large part, more than one third of the mutagenic potential of ambient air, is attributable to NPAHs.

Here, we try to advance knowledge of NPAHs by providing a fast, artifact-free measurement method for NPAHs and PAHs, which will allow investigating NPAH formation, degradation and sorption of NPAH from PAH on aerosol particulate matter under controlled conditions in a flow reactor, simulating an automotive exhaust system, and direct, artifact-free study of NPAHs and PAHs in the field. The common approaches for the measurement of PAHs and NPAHs are based on filter sampling and off-line chromatography. Artifact formation of NPAH from PAH collected on the filter and oxidative destruction of NPAH during sampling needs to be excluded, but no established method is available.

Photofragmentation (PF), the fragmentation of molecules by single- or multiphoton interaction, is employed in different modes since the 1980s. Different modalities can be distinguished, regarding the fragmentation mechanism and the way of fragment detection. High sensitivities in the low ppb or even ppt range for gas phase analysis can be achieved. Resonant fragmentation allows for a rather straight-forward system set-up; a single laser pulse can be employed for fragmentation and photoionization. Depending on the photon energy employed for the fragmentation, the fragments can be generated in an excited state. The excitation energy is released by optical emission, an effect sometimes addressed as PF/ fragment fluorescence, PF/ spontaneous emission, or PF/ prompt emission (PF/PE). Currently, we set up a system suitable for different of these methods in order to establish the fundamentals and the analytical figures of merit of the technique.

T. Bauch



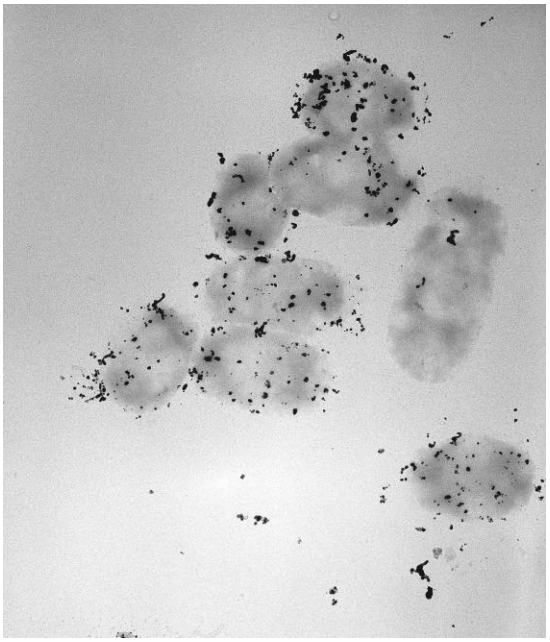
Experimental setup for photofragmentation experiments

Label-Free Detection of E. Coli by Using In situ Prepared Silver Nanoparticles

Funding: IWC, China Scholarship Council, Universitatea Babeş - Bolyai

The identification of bacteria is an important task in the light of the fact that many serious and even fatal medical conditions result from bacterial infection. The presence of Escherichia coli (*E. coli*) in drinking water, for example, usually indicates that other pathogen microorganisms could be also present. Surface-enhanced Raman spectroscopy (SERS) represents a powerful tool to identify bacteria, drawing from its high fingerprint (vibrational) information content, its extreme sensitivity (down to the single molecule level) and its obliviousness to the aqueous environment intrinsic to biological systems.

The SERS technique requires that the analyte is in close proximity to the nanoscale metallic surface in order to attain a high enhancement. Deposits of silver nanoparticles can be generated selectively inside or on bacteria in a controlled manner. An effective, facile and innovative method to produce silver nanoparticles as SERS substrates ("wall colloid") is here reported. The silver coating on the cell wall is achieved by soaking the *E. coli* solution with hydroxylamine hydrochloride and then adding the silver nitrate solution by gentle stirring. In addition to its great sensitivity, this in situ prepared substrate proved also a reliable selectivity, by discriminating between living and dead cells. In the case of dead *E. coli* we could observe the lack of enhancement of the specific cell wall vibrations. Therefore, this procedure is able to distinguish between living, active bacteria and inactive, dead ones.



TEM image of E. coli covered with SERS-active colloids

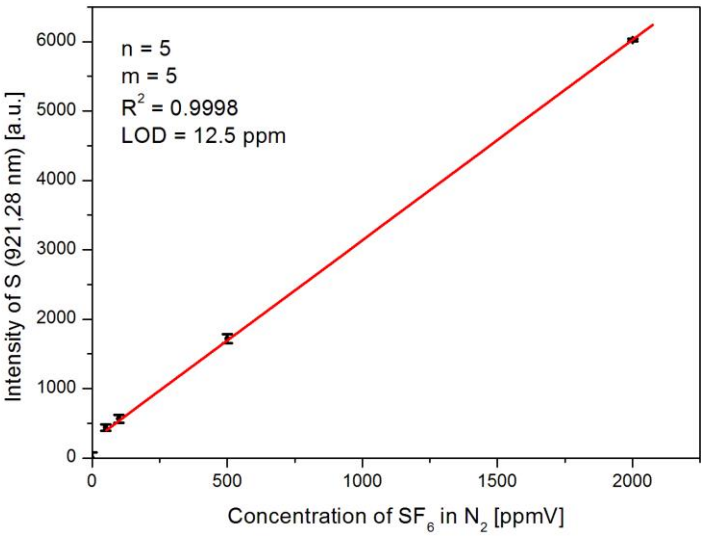
In order to obtain reproducible results, the volume-ratio of the analyte to colloidal particles, the influence of nanoparticles zeta potential, the time-dependent behavior of colloidal-bacterial suspension as well as different bacteria cultivation procedures were investigated and successfully optimized. The limit of detection for SERS measurements was found to be 10^3 cell/mL for living bacteria.

H. B. Zhou, N. E. Mircescu

Laser Induced Breakdown Spectroscopy as Detection Method of Trace Components in Biogas

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

Molten Carbonate Fuel Cells (MCFC) are promising alternative energy sources especially 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 sulphur compounds, halogenated hydrocarbons, and siloxanes. These contaminants cause undesired reactions at the anode and cathode, which reduce efficiency and lifetime of the cell.



Calibration curve of the LIBS system for sulfur

In this project, we are responsible for the development of the continuous monitoring of contaminations in biogas by laser induced breakdown spectroscopy (LIBS), an atomic emission spectroscopy based 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 Figure). 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. Currently, our focus is set on the identification of possible molecule fragmentation of the biogas, such as methane, carbon dioxide and nitrogen, but also larger organic molecules. They form the matrix of the analytes and can, as spectral interferences, influence substantially the measurements substantially.

For the next project phase, a spectrometer was bought which has two different light entrances that allows combining LIBS and Raman spectroscopy. 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

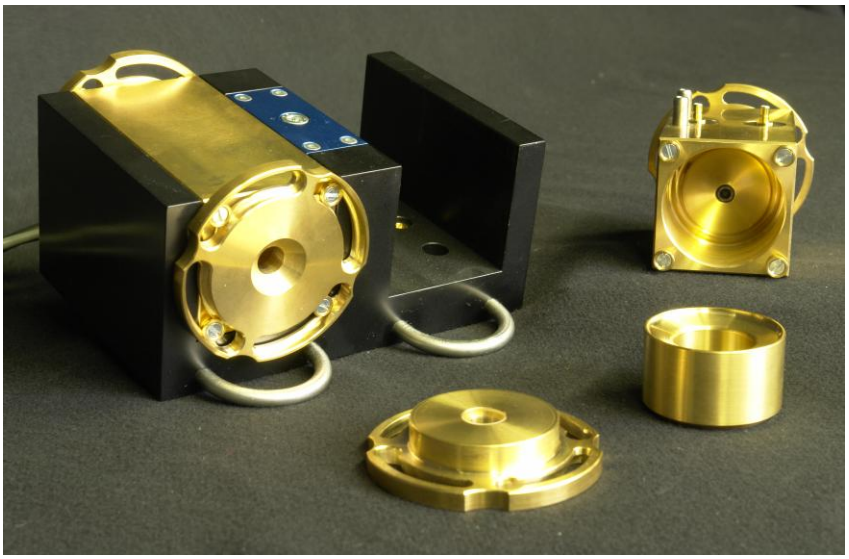
Photoacoustic Quantification of N_2O in Atmosphere and Exhaust Gas

Funding: IWC;
Cooperation: Nanoplus GmbH

The concentration of climate-relevant trace gases in the atmosphere is rising every year. Trace gases like nitrous oxide (N_2O) increase the greenhouse effect and contribute to the depletion of the ozone layer. One anthropogenic source for climate-relevant trace gases is the exhaust gas of combustion engines. A suitable measurement system could help to decrease the output and prevent further pollution. Photoacoustic (PA) spectroscopy has proven to be a very sensitive method for gas analysis. The principle of PA spectroscopy is the conversion of absorbed light energy into acoustical waves which can be detected by means of a microphone. The robustness and simplicity of some PA techniques allow for in situ monitoring. A typical PA setup contains of a laser, a PA cell, a microphone and a lock-in amplifier. The cell design can be modified to optimize the signal-to-noise ratio. Resonant cell designs, like Helmholtz resonant cells, can be used in PA systems and achieve high amplification factors. Combined with differential lock-in amplification a highly sensitive detector system is possible.

The aim of this research is to build a detector system dedicated to in situ exhaust gas detection of N_2O. According to the spectroscopic data of N_2O, a DFB infrared laser was chosen. The main part of the research is devoted to the design and the optimization of the detector system. Different resonant cell designs and new techniques like tuning-fork-enhanced detection are investigated.

C. Berger



Details of the PA cell currently used for the N_2O detection

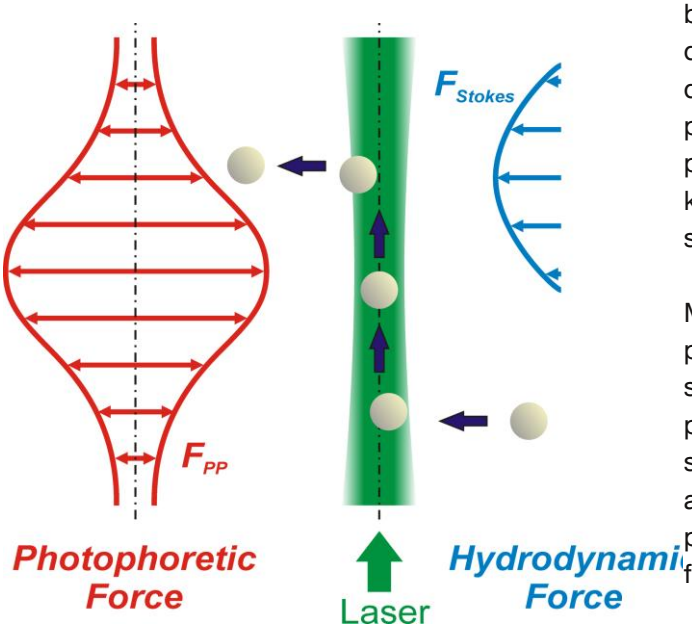
Photophoretic Separation of Hydrocolloids

Funding: DFG (Deutsche Forschungsgemeinschaft)

Multiparameter analysis of particles is essential for the clarification of origin and faith of particles in environmental, geological and chemical processes. A simultaneous characterization of physical and chemical parameters is often desired but often requires elaborate technical instrumentation for particles.

The application of optical forces on suspensions is a new approach for characterization and separation of colloid matter according to size and or refractive index. In photophoresis, particles are manipulated by the exchange of momentum between photons and microparticles. In order to induce migration in microparticles, a sufficient large photon flux is needed which was provided by a 1.7-W cw Nd:YAG laser. As the interaction of light depends on optical parameters, the photophoretic migration can be used for sizing of particles as well as separation according to refractive index. Within the project, a photophoretic bench-top separation system was realized. By a microfluidic system the dispersion is formed into a beam of approx. 300 µm in diameter.

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.



Princple of photophoretic separation

Using the Munich photophoretic particle sorter (MPPS 1) a polydisperse sample of 4.8-µm and 9.6-µm PS particles was fractionated.

Photophoretic particle sorting is contact free and does not require any auxiliary information such as fluorescence. The separation principle can be applied for bioparticles, e.g. bacteria and cells as well as inorganic particles with micron- and sub-micron dimensions.

C. Helmbrecht

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

Raman and SERS Analysis in Aqueous Environment: Focus on Stable Isotope Measurements of Microorganisms

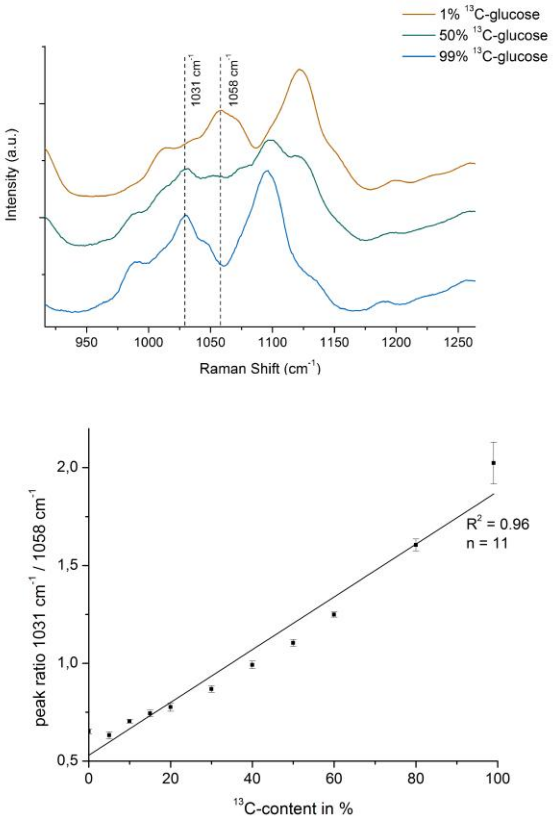
Funding: HelmholtzCentre Munich (Watter Alliance)
Cooperation: Institute of Groundwater Ecology, HelmholtzZentrum münchen

In natural environment microbial cells are normally found to be closely associated with interfaces, in the form of biofilms. Biofilms are communities of microorganisms (bacteria, protozoa, algae und fungi) embedded in a matrix of extracellular polymeric substances (EPS, biopolymers such as polysaccharides, proteins, nucleic acids, and humic-like substances). In aquatic systems biofilms may have a significant impact on the flux and fate of water quality-related substances. Since biofilms are very sensitive to varying boundary conditions, a rapid analytical tool for chemical characterization with high spatial resolution and sensitivity is required. Raman Microspectroscopy (RM) is a nondestructive technique providing in situ whole organism vibrational fingerprints for microbiological samples in the µm-range.

This vibrational spectroscopy allows non-invasive acquisition of Raman spectra without water interference. However, the quantum efficiency of the Raman effect (10^{-6} - 10^{-8}) and therefore the RM sensitivity is rather limited. However, the intensity of the Raman bands can be significantly increased if a molecule is attached to, or in immediate proximity of a nanometer-roughened metal (e.g. Ag or Au) surface. This technique, known as Surface-Enhanced Raman Scattering (SERS), results in enhancement factors in the range of 10^3 - 10^6 (up to 10^{14} at so called ”hot spots”) due to the electromagnetic (Surface Plasmon Resonance) and chemical enhancements (Charge Transfer Complex).

For better understanding of degradation pathways of water quality-related substances, stable isotopes (i.e. ^{13}C-tracer) are planned to be used as markers. It is already known that the Raman bands of proteins or nucleic acids in ^{13}C-labeled microorganism show a characteristic red shift in the Raman spectrum. As a first step *E. coli* cells with a varying content of ^{13}C were studied with normal Raman and SERS. In addition to the analysis of the *E. coli* cells, the characterization of glucose mixtures with different ratios of ^{12}C- and ^{13}C-glucose was performed, in order to obtain calibration curves on the basis of the ratio of the red shifted peaks.

P. Kubryk, N. P. Ivleva

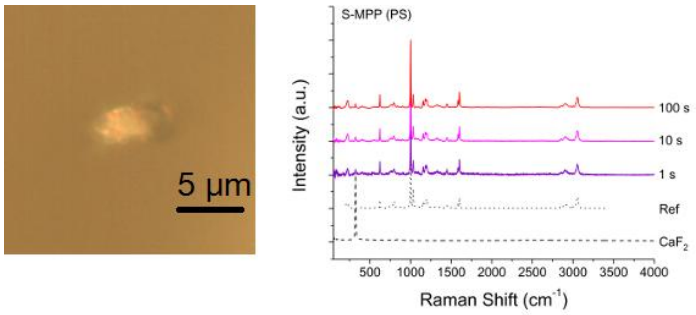


Red shift of ^{13}C-glucose in comparison with ^{12}C-glucose (A); Relation between red shift ratios calculated as intensity at 1031 cm^{-1} / intensity 1058 cm^{-1} of the analyzed glucose mixtures with different ^{13}C-content (B)

Identification and Quantification of Plastic Particles in Sediments of Aquatic Environment by Raman Microspectroscopy

Funding: DFG (Deutsche Forschungsgemeinschaft)
Cooperation: Prof. Dr. Laforsch, Univ. Bayreuth; H. Imhof, LMU Munich

Plastic is indispensable in our daily life. The production of plastic products increased immensely, from about 1.5 million tons in 1950 to 265 million tons in 2010 worldwide. Due to this development, plastic has become the fastest growing segment of the municipal waste stream. In recent years the pollution of marine environments with plastic waste has been reported. High amounts of plastic particles accumulate in the sediments and in the pelagic zone and can be ingested by many organisms. Thus, the plastic particles can accumulate in the food chain and pose a risk to the environment and human health. At the same time, the impact of plastic on aquatic ecosystems is not yet fully understood. The first important step to assess possible consequences of plastic debris in aquatic ecosystems is to perform quantification of plastic waste. We developed and verified a novel method to quantify plastic particles of different types and size classes, which is based on separation in dense (1.6 - 1.7 kg/L) fluids and employs identification by Raman Microspectroscopy (RM).



Optical microscope image and Raman spectra of a small micro-plastic polystyrene particles

RM provides vibrational fingerprint spectra of plastic and other (in)organic compounds with spatial resolution of an optical microscope. This technique allows us to analyze different types and size classes (macro-plastic, MPP >5 mm; large micro-plastic particles, L-MPP 1 – 5 mm; small micro-plastic particles, S-MPP <1 mm) of plastic separated from the sediment. In particular, we focused on the identification of particles in the size range of several microns, since these ecologically relevant particles have not been taken into account by studies of plastic debris in aquatic ecosystems. We found that even 1 s acquisition time can be sufficient for the identification of such particles (see figure). We also proved that, in addition to fresh plastic particles RM is well suited for the characterization of weathered and biodegraded particles. Furthermore, the analysis of cored plastic particles showed that RM allows us to identify plastic and included pigment(s). Thus, a combination of the particle separation from sediment with the identification by RM enables quantification of fresh, weathered, biodegraded, and colored plastic particles down to micron-size range. The next essential step would be to quantify plastic debris in sediment from different aquatic ecosystems.

J. Schmid, N. P. Ivleva

Bioseparation and Microarray Technology (Dr. M. Seidel)

Multiplex - Immunoassay for *Legionella pneumophila*

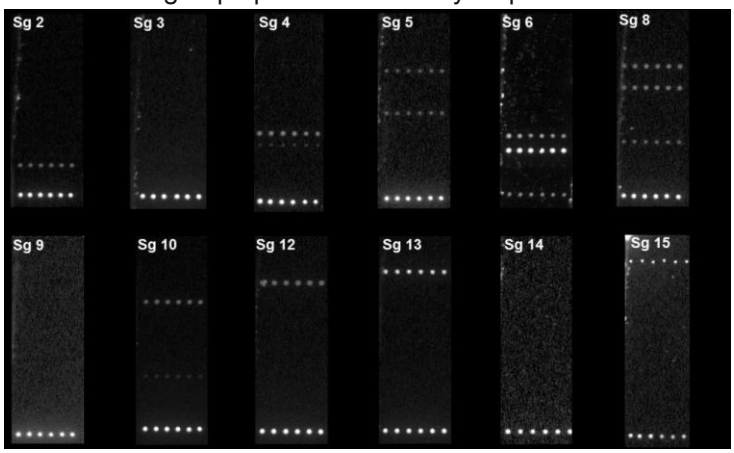
Funding: *IWC*
Cooperation: Bayerisches Landesamt für Gesundheit und Lebensmittelsicherheit; Prof. Lück, TU Dresden

Legionella spp. can cause pathogen infections like Pontiac Fever and Legionnaires disease. They are ubiquitous in small numbers in natural aquatic systems. At elev-elevated temperatures, as in hot water systems in buildings, factories or ships *Legionella* have ideal growth conditions due to thermotolerance and the existence of biofilms. Humans can be infected by inhaling contaminated aerosols, originating, e.g., from showers, cooling towers, evaporative cooling systems on the top of big buildings, or spa baths. Therefore, the analysis of pathogenic *Legionella* in bioaerosols is highly significant and important for the environmental hygiene.

L. pneumophila serogroup 1 is qualified as one of the most important epidemic serogroup, accounting for more than 80% of all counted legionnaire's diseases. However, this pathogen has additionally 14 serogroups, which are usually not detected as no commercial immunoassay can discriminate between these serogroups.

Microarray technologies like the Munich Chip Reader MCR3 are a promising technique for the fast identification and quantification of *L. pneumophila*. Sandwich microarray immunoassays offer advantages because they are able to perform the multiplexed analysis in a short time. The capture antibodies for each serogroup are immobilized covalently on the microarray chip by microcontact printing.

In a first screening of serogroup specific antibodies we have qualified monoclonal antibodies for serogroup 2, 4, 10, 12, 13, and 15 as highly specific. For the other serogroups we have found antibodies with cross activity to other serogroups or no activity. In the future, the screening for all *L. pneumophila* serogroups will be enforced to establish a serogroup specific microarray chip.

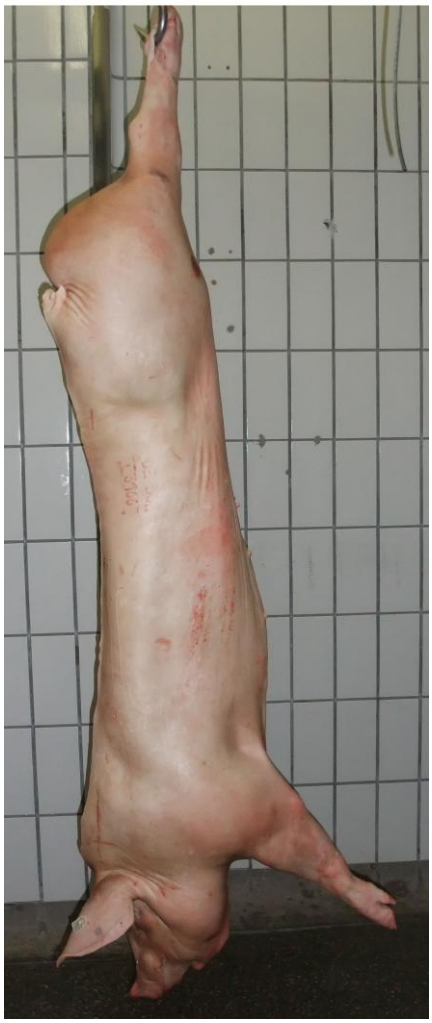


Antibody-screening of *L. pneumophila* serogroups

In a proof-of-concept study, bioaerosol samples from a shower and an evaporative cooling system were collected by a wetted-wall cyclone Coriolis µ. We have found antigens of *L. pneumophila* serogroup 1 which were not identified by the standard cultivation method. Further experiments are needed to evaluate the full potential of our sandwich microarray immunoassay for the quantification of *L. pneumophila* in the air.
A. Wunderlich, 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



Zoonose microarray analysis of slaughtered pig meat juice

Zoonosis is an infectious disease 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. At the moment, only the screening for Salmonella and Trichinella is regulated by law. Hence multiplexed and simultaneous monitoring of various pathogenic microorganisms would support the meat-processing industry to maintain high hygiene standards.

In this project, a method for fast and multiplexed detection of antibodies against zoonotic microorganisms in serum or meat juice samples of pigs for slaughter is to be developed.

To achieve 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 present zoonoses antibodies, these antibodies bind on the chip surface and can be detected by horseradish peroxidase (HRP)-labelled secondary antibodies. The chemiluminescence readout via CCD camera is performed on the microarray chip reader platform MCR 3 which combines the flow-through principle with the microarray technology. Using this method, incubation times are considerably reduced compared with ELISA test formats performed in titer plates or Line Blots. Moreover, multiple analytes can be detected simultaneously.

Up to now, we have successfully established a microarray immunoassay for principle studies on the target analyte of IgG antibodies formed against Hepatitis E virus. Within an assay time of 7 minutes we can detect HEV antibodies in real serum samples. Furthermore, we have achieved dose-response curves and screened a panel of sera samples based on three analytical methods (recomLine HEV, ELISA, and microarray) in comparison.

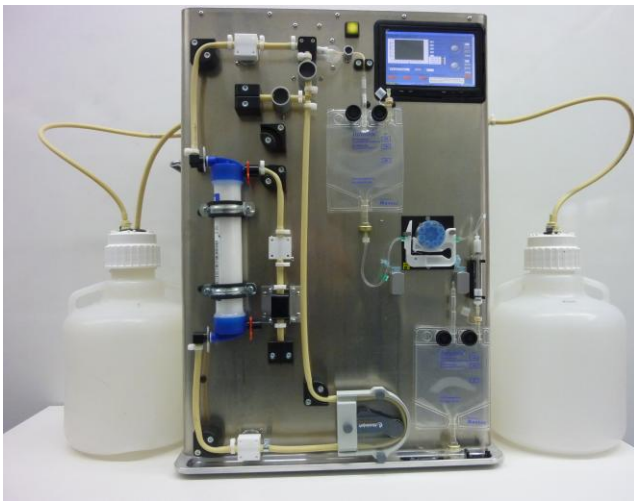
To finalise the project, the microarray is to be extended by antigens against other zoonotic agents.

K. Wutz , V. Meyer

Multiplexed Analysis of Pathogens and Indicator Organisms in Water – Combining Rapid Concentration Methods with Microarray Technology

Funding: BMBF (Federal Ministry for Education and Research; 02WU1142, PATH$_2$OGENSCAN)
Cooperation: Technologiezentrum Wasser, Landesgesundheitsamt Baden-Württemberg, GWK Präzisionstechnik GmbH

The quantification of waterborne pathogens (viruses, bacteria and parasites) at low concentrations demands rapid and efficient concentration methods which are compatible to cell cultivation assays or bioanalytical detection methods (e.g. qPCR, DNA microarrays, or immunoassays) dealing with sample volumes in the milli- or microliter range. These methods are important for studying the pathogen content in drinking water or raw water, for monitoring purposes, and for risk assessment. We have built up a new instrumentation for rapid and automated concentration of microorganisms and viruses, the Munich Microorganism Concentrator (MMC 3). In a first step all particles larger than 2 nm are rapidly concentrated by crossflow ultrafiltration using a dialysis membrane. Water samples are filtrated with a flow rate of 0.7 L/min. The concentrated particle fraction is eluted in a sterile bag which contains, depending on the water source, a broad range of microorganisms and viruses. As second concentration step a new adsorption - elution methods called monolithic affinity filtration (MAF) is applied. The MAF column consists of a hydrolyzed macroporous epoxy-based polymer. High recoveries were achieved by MAF columns for the bacterial virus (bacteriophage) MS2 112 (±16)% as model organism. Bacteriophages MS2 were spiked in 10 L tap water resulting in concentrations between 10^1 and 10^5 PFU/L. They were concentrated with the MMC 3 instrument in 33 min. The eluate has had a final volume of 1 mL. The recovery was determined by plaque assay and was between 42 and 50%. Also ground water was tested. The detection limit of a reverse transcriptase qPCR was improved from 10^4 GU/mL to 20 GU/mL. The aim of the project is to identify water-relevant pathogens and indicator organisms. Therefore, qPCR was established for noroviruses, adenoviruses, bacteriophage MS2, bacteriophage PhiX174, *E. coli*, *E. faecalis*, *Legionella sp*., Giardia, and Cryptosporidia. Especially the cross reactivities were optimized to analyze this set of contaminants on a multiplex microarray analysis platform (MCR 3 SLT). Therefore, the MCR 3 system was reconstructed for DNA microarray analysis. A temperature-controlled microarray cell was implemented to achieve optimized hybridization conditions for a sensitive and selective multiplex analysis.



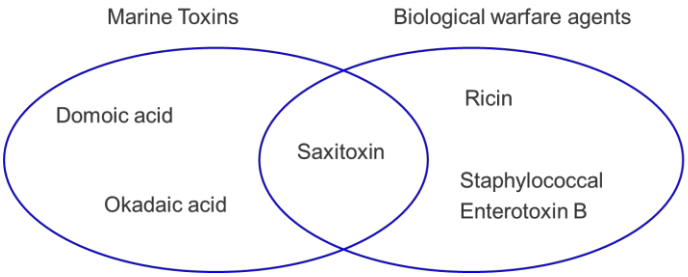
Munich Microorganism Concentrator (MMC 3)

S. Lengger, M. Rieger, L. Pei

Marine Toxin Microarrays & Biotoxin Microarrays

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

A novel multiplexed immunoassay for fast analysis of phycotoxins in shellfish samples has been developed. Therefore, a regenerable chemiluminescence (CL) microarray was established which is able to analyze automatically three different phycotoxins (domoic acid (DA), okadaic acid (OA) and saxitoxin (STX)) in parallel on the analysis platform MCR3. As a test format an indirect competitive immunoassay format



Biotoxin analysis for food safety and biosecurity

was applied. These phycotoxins were directly immobilized on an epoxy-activated PEG chip surface. After the competitive reaction, the CL signal was recorded by a CCD camera. Due to the ability to regenerate the toxin microarray, internal calibrations of phycotoxins in parallel were performed using the same microarray chip, which was stable for 25 consecutive measurements. For the three target phycotoxins multi-analyte calibration curves were generated in extracted shellfish matrix and in PBS buffer with LODs of 1.2 ± 0.6 µg/L for DA, 1.3 ± 0.5 µg/L for OA and 1.0 ± 0.2 µg/L for STX. For determination of toxin recoveries, the observed signal loss in the regeneration was corrected. After applying mathematical correction spiked and contaminated shellfish samples were quantified with a high accuracy in 20 min. This is the first demonstration of an antibody based phycotoxin microarray.

For the application of rapid screening of biological warfare agents (STX, S. aureus toxin B (SEB), and ricin) an indirect competitive immunoassay and a sandwich immunoassay are combined for the multiplexed analysis on the MCR 3. Therefore, an anti-idiotypic antibody is implemented for the quantification of STX who is immobilized on an antibody microarray chip together with capturing antibodies for SEB and ricin. For the multiplexed measurement detection antibodies and antigens were incubated for 1 min in a tube of the MCR3 before the mixture was flown over the antibody microarray chip. In 18 min a multiplexed analysis for each chip was possible with LODs of 2.9 ± 3.1 µg/L for ricin, 0.1 ± 0.1 µg/L for SEB and 2.3 ± 1.7 µg/L for STX, respectively.
A. Szkola

Pathogenic Viruses in Water – Detection, Transport and Elimination

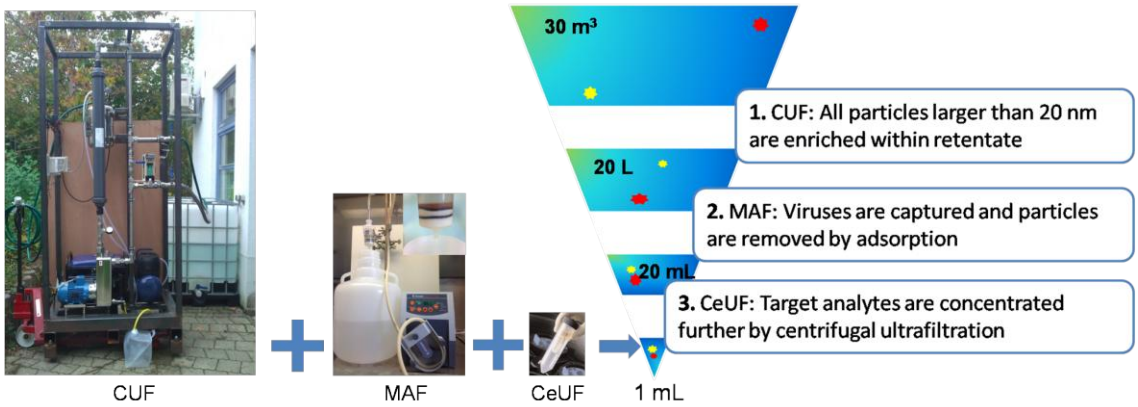
Funding: DFG (Deutsche Forschungsgemeinschaft), China Scholarship Council
Cooperation: Centre of Infectiology and Infection Prevention, University of Bonn; Federal Environment Agency, Berlin; Institute of Groundwater Ecology, Helmholtz Zentrum München; Institut für Siedlungswasserwirtschaft und Abfalltechnik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

In most cases, concentrations of viruses in the ambient environment are lower than detection limits of microbiological assays. However, viruses are 10 - 10,000-fold 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. As recommended, large water volumes (> 10 m^3) have to be analyzed to characterize the risk of waterborne viruses.

To meet these requirements, we designed a three-step enrichment system combining crossflow-ultrafiltration (CUF), monolithic affinity filtration (MAF), and centrifugal ultrafiltration (CeUF). After such three-step enrichment, viruses in 30 m^3 samples can be concentrated to 1 mL. CUF-Unit 1, having a power generator on board, can be set up on site. A maximum flow rate of 1724 L/h is achieved with a recovery rate of 45.4 (± 23.3)%. For MAF, a recovery of 106 (± 23)% is achieved for over 6 orders of magnitude (10^3 - 10^8 PFU) within 10 min with a enrichment factor of 500. Concentrating of MS2 bacteriophage spiked in 10 m^3 tap water to 1 mL was achieved by our system within 7 h with an enrichment factor of 2.4×10^5 and a recovery of 11.2 (± 3.1)%.

As a mobile system, it was also tested with ground water spiked with 0.01% sewage in the outdoor experimental channel at the Federal Environment Agency, Berlin. Although the high turbidity water matrix is really a huge challenge for this system which is designed for tap water, enrichment factors of 3.4×10^4 and 7.0×10^4 were found for human adenoviruses and murine noroviruses. The broad applicability of such combination system promises simultaneous enrichment of various organisms at the same time. In other words, the diversity of organisms in the original sample can be maintained in the final 1-mL eluate. This is important for following high-throughput detection methods, e.g. microarray technology.

L. Pei, M. Rieger, S. Lengger



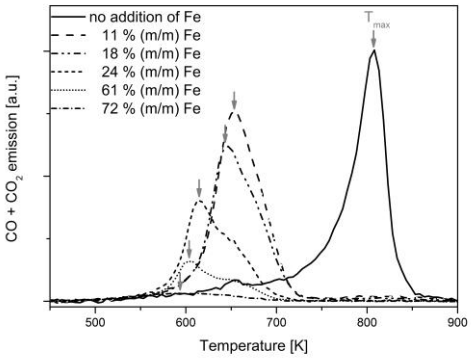
Work-flow of virus concentration in 30 m^3 samples of drinking water

Aerosol Research (Prof. Dr. R. Niessner)

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

Funding: DFG (Deutsche Forschungsgemeinschaft), RFBR (Russian Foundation of Basic Research)
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 ironpentacarbonyl $Fe(CO)_5$ 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.



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

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.

H. Bladt, N. P. Ivleva

Particle Number Measurement

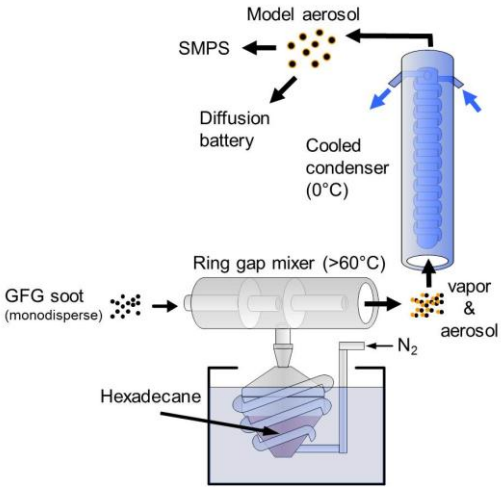
Funding: FVV (Association for Combustion Engine Research)
Cooperation: Institute for Internal Combustion Engines, TUM

Progressive tightening of regulations concerning emissions from diesel fueled vehicles resulted in limit values for particle mass and, recently, for the emitted particle number with a limit of $6 \cdot 10^{11}$ particles per cm^3 since 2011. Also, a regulation was set by the EU (Regulation 83) to define the instrumentation, prerequisites and sampling procedure used for its determination.

Within this regulation there are some aspects requiring further investigateion. One crucial aspect is the use of a condensation nuclei counter (CNC) as detection instrument. As the counting efficiency of the CNC strongly depends on the composition of the aerosol, the instrument may report different results for different types of aerosols. Therefore, the aerosol used for calibration is very important. Another critical aspect of the EU regulation is that only the solid particles in the exhaust gas are to be counted. The removal of the undesired volatile components from the exhaust gas is suggested to be carried out by thermal pretreatment (evaporation of the volatiles) and subsequent dilution (preventing re-condensation). It has to be clarified whether this treatment alters the physico-chemical properties of the aerosol particles and thus affects the counting efficiency of the subsequent CNC. Also, the complete removal of volatile layers from the particle's surface is questionable.

The aim of this project is to investigate the problems mentioned above that might occur during particle number measurement according to EU Regulation 83. For this investigation, different model aerosols like spark discharge soot coated with n-hexadecane, sulfuric acid and sodium chloride were generated to mimic diesel exhaust gas.

It could be shown that the counting efficiency is higher for some exhaust components, which are soluble in the working fluid of the CNC. For n-hexadecane coated soot the counting efficiency is up to 30 % higher in comparison to uncoated soot with the same particle size. Thus, the instruments do not meet the specified cut off values for this type of aerosol. By evaporation of the n-hexadecane the counting efficiency dropped back to the value of uncoated soot. Thus it can be concluded that a layer of hexadecane can be evaporated completely from the soot core but during the evaporation process, the core particle size was decreased to a small amount (diffusion battery measurements).



Instrumental setup for n-hexadecane coating of soot particles

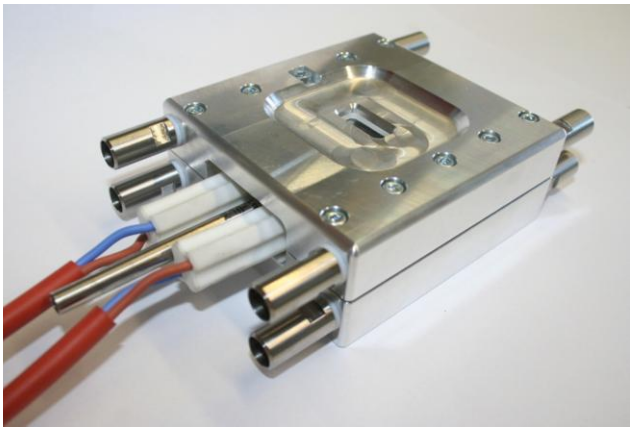
Additionally, CNCs from different manufacturers were compared by means of the generated model aerosols to evaluate the influence of varying calibration procedures and calibration aerosols on the counting efficiency. The response curves of the three tested instruments differed in shape, but still mostly met the limit values required by Regulation 83 for a pure soot aerosol.

B. Kiwull, J.-C. Wolf

Conductivity for Soot Sensing: Possibilities and Limitations

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

Aerosol particles have a significant influence on the climate, environment and human health. In urban areas especially soot particles emitted by diesel engines, pose a health risk. Current and upcoming limits require a removal of diesel soot particles, which is mainly accomplished by ceramic wall-flow diesel particle filters (DPF). To prevent increasing backpressure the DPF has to be regenerated periodically by gasification of the deposited soot. Thereby the efficiency of the regeneration step is affected by the oxidation reactivity of the deposited soot, which mainly depends on the nanostructure of the soot particles. Since the DPF has to be controlled to avoid malfunctions, cheap and reliable tools are demanded for an on-board diagnostic system (OBD).



Picture of heatable flow cell

A very promising attempt is the detection of particles by a conductometric sensor. As the conductance is strongly affected by the nanostructure, which opens the possibility to use the conductometric sensor method also as a simple cheap and rapid analytical tool for characterization of soot structure.

In this study we investigate the possibilities and the limitations of the electrical conductivity measurement for soot sensing. So far we demonstrated the functionality of the sensor principle (based on measuring the electrical resistance of deposited particles between interdigitated electrodes) under real life conditions and by laboratory studies. Now the focus was on the influence of NO_2 on the sensor response of a loaded sensor under various temperatures. With our test-bench experiments we could demonstrate the sensitivity of the soot-loaded sensor to different NO_2 concentrations, which can be attributed to oxidation of the soot surface. This knowledge opens the possibility of a third detectable parameter by this sensor principle beside the nanostructure analysis and particle detection.

A second approach was to develop a device which makes it possible to investigate the influence of the nanostructure and the oxidation behaviour of soot on the electrical conductivity combined with the monitoring of the processes by the Raman microspectroscopy and the temperature programmed oxidation in one setup.

Therefore, we developed a flowcell which can be heated up to 1000 °C and can be placed under the Raman microscope, due to a good isolation and a effective cooling of the cell frame. Through a quartz window it is possible to observe the soot layer on the conductometric sensor inside the cell. On the outlet of the cell a FTIR can be plugged as a gas detector for the temperature programmed oxidation. The performance of the cell as well as the idea of combining all the analytical tools for soot structure analysis used in this project in one single setup is now proven.

B. Grob, J. Schmid

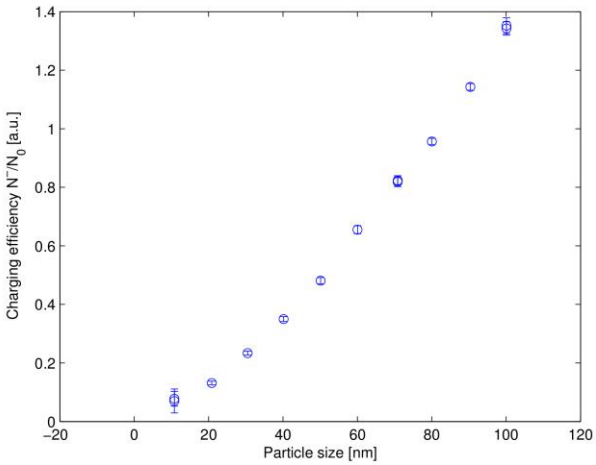
Indirect Photoelectric Diffusion Charging of Aerosols

Funding: IWC

Black carbon has a big impact on the public health as well as to the climate. Therefore the upcoming exhaust emission standards Euro 5b and 6 for diesel engines include a limit of 6×10^{11} particles/km of non-volatile particles. To measure the particle emission of engines, complicated measurement set-ups are necessary, which can handle high particle concentrations, prevent coagulation, separate non-volatile and volatile particles and count smallest particles efficiently. Currently condensation nucleus counters (CNC) are favored as analytical technique. CNCs, however, do have many drawbacks including the reproducibility and susceptibility to th chemical composition of the particles. Also, there is still no calibration standard as well as a standard method for monitoring the stability of the CNCs.

Alternatively, unipolar charged particles can be counted by an aerosol electrometer, which would represent a primary standard measurement. This requires a unipolar charging method is necessary, capable to charge particles in a size range of 10 to 100 nm. Such a setup could then be used as a reference for calibration and stability checks of CNCs.

The setup we use is based on a design published by Bucholski and Niessner in 1991, consisting of an elliptically grooved, electrically grounded aluminum block with an UV lamp fixed in one focus of the ellipse. The aerosol flux is pumped through a quartz tube placed in the second focus with a grounded metal grid on the inner surface. In the medial axis of the tube a metal rod is installed, where after applying a voltage electrons are emitted, due to the photoeffect. By means of diffusion the photoelectrons can charge aerosol particles directly or form negative ions by attachment processes, which then collide with the aerosol particles. It was shown that the set-up is working for NaCl particles, with a gold or nickel rod at a wavelength of 185nm with nitrogen as carrier gas, which is not suitable for soot particles, because the energy of the photons is larger than the work function of the particle surface. The limit for diesel soot particles would be photons with a wavelength of 254 nm. The ideal material has a lower work function and has to have a stable surface under the influence of oxygen. Due to this fact most of the metals are not suitable, because of surface oxidation. Instead, we are using a non-porous carbon, which is chemical inert and has a high electrical conductivity.



Calibration curve for the photo charger

The results so far indicate a very stable and efficient charging process. To prove the system we addressed the influence of the carrier gas composition, the particle size, the particle concentration and the effect of multiple charging. The experimental results suggest that indirect photoelectric diffusion charging can overcome the disadvantages of direct photoelectric aerosol charging and provides an alternative to the particle counting by a CNC.

B. Grob

Publications

Peer Reviewed Journals

D. Baumgardner, O. Popovicheva, J. Allan, V. Bernardoni, J. Cao, F. Cavalli, J. Cozic, E. Diapouli, K. Eleftheriadis, P.J. Genberg, C. Gonzalez, M. Gysel, A. John, T.W. Kirchstetter, T.A.J. Kuhlbusch, M. Laborde, D. Lack, T. Müller, R. Niessner, A. Petzold, A. Piazzalunga, J.P. Putaud, J. Schwarz, P. Sheridan, R. Subramanian, E. Swietlicki, G. Valli, R. Vecchi and M. Viana; Soot Reference Materials for Instrument Calibration and Intercomparisons: a Workshop Summary with Recommendations. Atmos. Meas. Tech. 5 (2012) 1869-1887

H. Bladt, J. Schmid, E. Kireeva, N. Persiantseva, K. Heister, M. Timofeev, J. Uihlein, O. Popovicheva, N. Ivleva, R. Niessner; Impact of Fe Content in Laboratory – Produced Soot Aerosol on its Thermo – Chemical Properties. Aerosol Science and Technology. 46 (2012) 1337-1348

T. Fässler, V. Hlukhyy, S. Ponau, S. Lidin, N. Ivleva and R. Niessner; Extreme Differences in Oxidation States: Synthesis and Structural Analysis of the Germanide Oxometallates. Inorg. Chem. 51 (2012) 4058-4065

B. Grob, J. Schmid, N. Ivleva, R. Niessner; Conductivity for Soot Sensing: Possibilities and Limitations. Anal. Chem. 84 (2012) 3586-3592

C. Haisch, R. Niessner; A Photoacoustic Analyzer for the Artifact-free Parallel Detection of Soot and NO2 in Engine Exhaust. Anal. Chem. 84 (2012) 7292-7296

H. Imhof, J. Schmid, R. Niessner, N. Ivleva and C. Laforsch; A Novel, Highly Efficient Method for the Quantification of Plastic Particles in Sediments of Aquatic Environments . Limnology and Oceanography: Methods 10 (2012) 524-537

X. Karsunke, H. Wang, E. Weber, M. McLean, R. Niessner, J. Hall and D. Knopp; Development of Single Chain Variable Fragment (scFv) Antibodies Against the Hapten Benzo [a] pyrene: A Binding Study. Anal. Bioanal. Chem. 402 (2012) 499-507

M. Knauer, N. Ivleva, R. Niessner and C. Haisch; A Flow – through Microarray Cell for the Online SERS Analysis of Antibody – captured E. coli Bacteria. Anal. Bioanal. Chem. 402 (2012) 2663-2667

V. Langer, G. Hartmann, R. Niessner and M. Seidel; Rapid Quantification of Bioaerosols Containing L. pneumophila by Coriolis µ R Air Sampler and Chemiluminescence Antibody Microarrays. J. Aerosol Sci. 48 (2012) 46-55

X. Liu, M. Gonzalez, R. Niessner and C. Haisch; Strong Size – dependent Photoacoustic Effect on Gold Nanoparticles: a Sensitive Tool for Aggregation – based Colorimetric Assays. Analytical Methods. 4 (2012) 309-311

P. Menzenbach, H. Bladt, R. Nießner and C. Haisch; A Wide-range Photoacoustic Aerosol Absorption Spectrometer. Anal. Chem. 84 (2012) 8941-8945

L. Pei, M. Rieger, S. Lengger, C. Zawadsky, A. Thiem, R. Niessner, M. Seidel; Combination of Crossflow Ultrafiltration, Monolithic Affinity Filtration, and Quantitative Reverse Transcriptase PCR for Rapid Enrichment and Quantification of Bacteriophage MS2 in

Environmental Water. Environmental Science & Technology 46 (2012) 10073-10080
O. Popovicheva, E. Kireeva, N. Persiantseva , M. Timofeev, H. Bladt, N. Ivleva, R. Niessner and J. Moldanová; Microscopic Characterization of Individual Particles in Multicomponent Ship Exhaust. Journal of Environmental Monitoring 14 (2012) 3101-3110
M. Rieger, G. Schaumann, Y.K. Mouvenchery, R. Niessner, M. Seidel and T. Baumann; Antibody – labeled Nanoparticles for the Visualization of Surface – immobilized Benzo[a]pyrene Using NMR Relaxometry and Magnetic Resonance Imaging. Anal. Bioanal. Chem. 403 (2012) 2529-2540
M. Saini, M. Taggart, D. Knopp, S. Upreti, D. Swarup, A. Das, P. Gupfa, R. Niessner, V. Prakash, R. Mateo and R. Cuthbert; Detecting Diclofenac in Livestock Carcasses in India with an ELISA: a Tool to Prevent Widespread Vulture Poisoning. Environ. Poll. 160 (2012) 11-16
J. Tang, D. Tang, R. Niessner, D. Knopp and G. Chen; Hierarchical Dendritic Gold Microstructure – based Aptasensor for Ultrasensitive Electrochemical Detection of Thrombin Using Functionalized Mesoporous Silicea Nanospheres as Signal Tags. Anal. Chim. Acta 720 (2012) 1-8
B. Tilley & T. Baumann, On Temperature Attenuation in Open-loop Wells. Renew. Energy 48, (2012) 416-423.
P. Völk, G. Wachtmeister, G. Hörnig und R. Niessner; Ablagerungsmechanismen in Abgaswärmetauschern. Motortechnische Zeitschrift 73 (2012) 710-717
J.C. Wolf and R. Niessner; High Capacity NO_2 Denuder Systems Operated at Various Temperatures (298 K – 473 K). Anal. Bioanal. Chem. 404 (2012) 2901-2907
Y. Wang, H. Yang, M. Pschenitza, R. Niessner, Y. Li, D. Knopp; Highly Sensitive and Specific Determination of Mercury (II) in Water and Food Samples with an ELISA Based on a Novel Monoclonal Antibody. Anal. Bioanal. Chem. 403 (2012) 2519-2528
C. Würth, M. Gonzales, U. Panne, R. Niessner, C. Haisch and U. Resch – Genger; Determination of the Absolute Fluorescence Quantum Yield of Rhodamine 6G with Optical and Photoacoustic Methods – Providing the Basis for Fluorescence Quantum Yield Standards. Talanta 90 (2012) 30-37
H.-W. Yu, I.S. Kim, R. Niessner, D. Knopp; Multiplex Competitive Microflow Immunoassay Using Quantum Dot Fluorescent Labels. Anal. Chim. Acta 750 (2012) 191-198
B. Zhang, B. Liu, D. Tang, R. Niessner, G. Chen and D. Knopp; DNA-based Hybridization Chain Reaction for Amplified Bioelectronic Signal and Ultrasensitive Detection of Proteins. Anal. Chem. 84 (2012) 5392-5399

Conference Presentations

Oral Presentations

T. Baumann, N. P. Ivleva, C. Metz, M. Rieger & R. Niessner, Visualization of biogeochemical interfaces using micromodels and MRI, INTERPORE 2012, 14.-16.5.2012, West Lafayette, U.S.A.

T. Baumann, S. Huckele, M. Reitzel & R. Niessner, Nanoparticles in the aquatic environment, INTERPORE 2012, 14.-16.5.2012, West Lafayette, U.S.A.

T. Baumann, Der Orientierungsrahmen Für die ursprüngliche Reinheit, Jahrestagung ARGE Naturwissenschaft und Technik im VBK, 19.5.2012, Bad Arolsen.

B. Grob and R. Niessner, Indirect Photoelectric Diffusion Charging of Aerosols, EAC 2012, 02. - 07.09.2012, Granada, Spain.

C. Haisch, Optothermal Effects: Future Potential of an Old Technique, GDCh Vortragsreihe der Ortsgruppe Regensburg, 23.07.2012, Regensburg, Germany.

C. Haisch, Optothermal Effects: New Applications of an Old Technique, Analytica Conference, 1.-4. 04. 2012, Munich, Germany (Bunsen-Kirchhoff award presentation).

C. Haisch, News on Photoacoustics in Exhaust Monitoring, 7. Internationales Forum Abgas- & Partikelemissionen, 6.-7. 03. 2012, Ludwigsburg, Germany.

C. Haisch, TwinPAS – A Photoacoustic Instrument for the Parallel, Time-Resolved Analysis of Soot and NO_2 in Exhaust Gas, EAC 2012, 4. 09. 2012, Granada, Spain.

M. Herbrich, N. Frank, C. Pletl, F. Barenth & T. Baumann, Monitoring zur Minimierung der Risiken bei Planung und Betrieb tiefengeothermischer Anlagen im Malmaquifer, Workshop Betriebsbegleitendes Fluidmonitoring in geothermischen Anlagen, 26.3.2012, Potsdam.

M. Herbrich, N. Frank, C. Pletl, F. Barenth, R. Baasch, R. Niessner & T. Baumann, Minimierung von Risiken bei Planung und Betrieb tiefengeothermischer Anlagen im Malmaquifer, Der Geothermiekongress, 13.-16.11.2012, Karlsruhe.

M. Lafogler, R. Baasch, F. Wenderoth, U. Steiner, A. Schubert, R. Niessner & T. Baumann, Quantifizierung und Prognose des Malmaquifer-Reservoirs mit einem Push-pull-Test in Pullach, Der Geothermiekongress, 13.-16.11.2012, Karlsruhe.

M. Seidel, S. Lengger, L. Pei, S. Wieghold, J. Otto, O. Schneider, F. Hauke, C. Heese, A. Tiehm, J. Fleischer, I. Schechter, R. Armon, R. Niessner, Rapid microbiological water quality monitoring based on polymeric imprinted enrichment coupled to spectral inspection and microarray technology, German-Israeli cooperation in water technology research, 12th Status Seminar 2012, 17-18 October 2012, Haifa, Israel.

Poster Presentations

T. Baumann, S. Huckele & R. Niessner, Nanoparticles at the interface between atmosphere and hydrosphere, EGU General Assembly, 23.-27.4.2012, Vienna.

T. Czymai, C. Habel, K. Kloth, C. Baumgartner, R. Dietrich, E. Märtlbauer, M. Seidel, R. Niessner, Qualifying and Quantifying Antibiotic residues in Raw Milk, Euroresidue VII, 14-16.5.2012, Egmond aan Zee, The Netherlands.

B. Grob, J. Schmid, N.P. Ivleva and R. Niessner, Conductivity for Soot Sensing: Possibilities and Limitations, EAC 2012, 02. - 07.09.2012, Granada, Spain.

C. Haisch, Time-resolved NO2 Analysis in the Presence of Soot, EAC 2012, 4.09.2012, Granada, Spain.

M. Herbrich, N. Frank, C. Pletl, R. Niessner & T. Baumann, Fluid monitoring of geothermal facilities in the Bavarian molasse basin, FH-DGG Tagung, 16.-19.5.2012, Dresden.

M. Lafogler, L. Pang, M. Close, R. Niessner & T. Baumann, Phosphorous transport, EGU General Assembly, 23.-27.4.2012, Vienna.

M. Lafogler, M. Nottebohm, F. Wenderoth, R. Baasch, A. Schubert, M. Sauter, R. Niessner & T. Baumann, Characterizing a geothermal doublet in the Malm aquifer of the Bavarian molasse basin by performing a push-pull tracer test, FH-DGG Tagung, 16.-19.5.2012, Dresden.

V. Langer, R. Niessner, M. Seidel, Antikörper-Mikroarrays als schnelles Multiplex-Verfahren zum Nachweis von L. pneumophila in Wasserleitungssystemen. WASSER 2012, May 2012, Neu-Ulm.

S. Lengger, L. Pei, M. Rieger, R. Niessner, M. Seidel, Fast Enrichment Techniques in Combination with Multiplexed DNA Microarray Analysis for Quantification of Viruses in Surface Water. WASSER 2012, May 2012, Neu-Ulm.

C. Metz, N. P. Ivleva, R. Niessner & T. Baumann, Bacterial growth in porous media - the pore scale perspective, Wasser 2012, 14.-16.5.2012, Neu-Ulm.

S. Oswald, R. Niessner & D. Knopp; Hapten Microarray-based Screening of Mycotoxins in Cereals. 34. Mycotoxin Workshop, 14.-16.05.2012, Braunschweig, Germany.

L. Pei, M. Rieger, S. Lengger, R. Niessner, M. Seidel, Fast and Efficient Enrichment of Viruses from 30-m3 Water by Combining Crossflow-Ultrafiltration and Monolithic Column. WASSER 2012, May 2012, Neu-Ulm.

M. Pschenitza, Y. Wang, H. Yang, R. Niessner, Y. Li, D. Knopp & A. Deng. Hochsensitive und spezifische Bestimmung von Quecksilber(II) in Wasser. Wasser 2012, Jahrestagung der Wasserchemischen Gesellschaft, 14.-16.05.2012, Neu-Ulm, Germany

A. Szkola, R. Niessner, M, Seidel, Multiplex-Nachweis zur Analyse von marinen Biotoxinen. WASSER 2012, May 2012, Neu-Ulm.

Scientific Committees

T. Baumann, Fate and Transport of Biocolloids and Nanoparticles in Soil and Groundwater Systems. EGU General Assembly, 23.-27.4.2012, Vienna (Co-convener)

Invited Lectures

T. Baumann, Heilbäder in der Provinz Krabi (Thailand), 3. Forum Gesundheitswirtschaft Bayern, 29.2.2012, Bad Kissingen.

T. Baumann, Geothermal Exploration of the Malm aquifer in the Bavarian Molasse Basin - Hydrochemical and Technical Issues, 17.4.2012, Institute of Engineering Geology, ETH Zürich.

T. Baumann, Colloids in Groundwater, 29.8.2012, Department of Earth Sciences, Utrecht University.

T. Baumann, Geothermal Exploration of the Malm Aquifer in the Bavarian Molasse Basin - Hydrochemical and Technical Aspects, 5.9.2012, Centre for Integrated Petroleum Research, University Bergen.

T. Baumann, Visualization of Processes in Porous Media, 5.11.2012, Institut für Erd- und Umweltwissenschaften, Univ. Potsdam.

T. Baumann, Geothermal Exploration in the Bavarian Molasse Basin - Hydrochemical Aspects, 6.12.2012, GeoForschungsZentrum Potsdam - Internationales Geothermiezentrum.

T. Baumann, Geothermal Exploration of the Malm Aquifer - Hydrochemical Analysis as Prerequisite for Exploration and Long Term Use, 5.12.2012, TUM Analytik Club.

D. Knopp, Bioanalytische Methoden zum Mykotoxinnachweis in Getreide: Gegenwärtiger Stand und Ausblick, Workshop Mykotoxine in Lebens- und Futtermitteln – ein ungelöstes Problem in der Qualitätssicherung, 26.09.2012, Dortmund.

C. Haisch, Nanopartikel als Ziel und Hilfsmittel analystischer und bioanalytischer Verfahren, 16.11.2012, Tübingen.

C. Haisch, Analytische Chemie von und mit strukturierten Proben, 12.11.2012, Münster.

C. Haisch, Structured Samples: Targets, Toys, and Tools in Spectroscopic Analysis, 12.01.2012, Regensburg.

R. Niessner, Microarray Technology for Rapid & Quantitative Analysis of Water, Air & Food Contaminants, 19.04.2012, ANALYTICA Conference München.

R. Niessner, Measurement Means Knowledge – New Tools (Needed) for Monitoring of Water Quality, 04.05.2012, Exploratory Workshop, TUM Institute for Advanced Studies, München.

R. Niessner, Soot Aerosol Pitfalls & Possibilities, 23.05.2012, Int. Assoc. Environ. Anal. Chem., Antwerpen.

R. Niessner, Characterization of Soot – Pitfalls and Possibilities, 07.09.2012, European Aerosol Conference, Granada.

R. Niessner, Chemical Characterization, 10.09.2012, Bilbao Talks on Aerosol Science, Aerosol Science and Technology at the Crossroads: New Problems and New Instruments, Bilbao.

R. Niessner, Measurement Means Knowledge – New Tools (Needed) for Monitoring of Water Quality, 12.10.2012, Institut für Analytische Chemie, Universität Regensburg.

R. Niessner, Mikroarrays als neue Möglichkeit der Wasserüberwachung, 09.11.2012, Engler – Bunte – Institut, TH Karlsruhe.

M. Seidel, Combination of Concentration Methods and Multiplexed Microarrays for the Rapid Quantification of Pathogens in Water, Young Water Talents Symposium, 1.7.2012, Singapore.

M. Seidel, Multiplex-Mikroarray-Analyse am Beispiel von Toxinen, Mikroorganismen und Viren, Robert-Koch-Institut, 27.4.2012, Berlin.

M. Seidel, Dem pathogenen Virus auf der Spur, LiveLab, Analytica 2012, 19.4.2012, München.

M. Seidel, Das Wasserlabor der Zukunft, LiveLab, Analytica 2012, 18.4.2012, München.

M. Seidel: Multiplex – Mikroarray – Analyse. Hochschulöffentlicher Vortrag im Rahmen des Habilitationsverfahrens, Lehrstuhl für Analytische Chemie, TUM, 15.2.2012, München.

M. Seidel, Multiplex microarray analysis in food and environmental samples, Queen's University, Belfast, UK.

Hydrochemical consulting

Mineralisation control analyses: Bad Abbach, Bad Aibling, Bad Birnbach, Bad Füssing, Bad Griesbach, Bad Gögging, Bad Reichenhall, Bad Rodach, Bad Wimpfen, 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 Abbach, Bad Aibling
Deep Hydrogeothermal Energy Exploration: Aschheim, Pullach, Sauerlach, Waldkraiburg

Theses

PhD Theses

Dipl. Phys. Karin Eilert-Zell: Characterization of a Combined Optoacoustic/Ultrasound System (OPUS) for Tomographic Absorption Measurements.
Dipl.-Ing. Gabriele Hörnig: Untersuchungen zur Aerosolabscheidung in AGR – Wärmetauschern.
MSc Chem. Veronika Langer: Nachweis von Legionella pneumophila in Luft und Wasser mittels Antikörper-Mikroarrays.
Dipl.-Chem. XiangJiang Liu: Nanoparticles and Surface-Enhanced Optical Effects for Chemical and Biological Sensing.
MSc Chem. Sonja Ott: Kombination von monolithischer Immunfiltration und Antikörper-Mikroarrays zur schnellen Quantifizierung von Mikroorganismen in Milch.
MSc Chem. Martin Rieger: Entwicklung von Anreicherungs- und Detektionsmethoden umwelt-relevanter Analyten (Viren in Trinkwasser; adsorbiertes B[a]P
MSc Chem. Johannes Schmid: Charakterisierung der partikulären Emission von Motoren: Reaktivität, Struktur und Leitfähigkeit von Dieselrußen.

M.Sc. Theses

BSc Chem. Michael Bauhofer: Analytical Method for Quantification of L. Pneumophila by Combination of Concentration Methods and Sandwich Microarray Immunoassay.
Cand. Phys. Christoph Berger: LED-induzierte Fluoreszenzsensorik zur Wasserüberwachung.
BSc Chem. Ruili Feng: Analysis of Energy Absorption Properties of Foams for Impact Protection Applications.
Cand. Chem.-Ing. Markus Hager: Auslegung eines Systems zur Beurteilung der diffusiophoretischen Abscheidung von Rußpartikeln in Anwesenheit von Wasserdampf.
BSc Chem. Maria Hübner: Entwicklung eines Glyco-Chips zur Detektion von Rizin.
BSc Chem. Bettina Kiwull: Untersuchungen zur Abtrennung flüchtiger Bestandteile aus Dieselabgas.
BSc Chem. Meera Mahle: Use of HPLC Coupled with High Resolution Mass Spectrometry for the Analysis of Environmental Samples.
BSc Ing.-Hydrogeol. Bastian Knorr: Colloid-associated Phosphorous Transport in Intact Vadose Zone Lysimeters of Coarse Sandy Gravels under Saturated Conditions.
BSc Maria Theresa Rock: Occurrence of Catecholamines and Other Biomarkers in Stressed and Nonstressed Amphipods.

BSc Geol. Wiss. Gabriella Somogyi: Charakterisierung der Wechselwirkung von Fluoreszenzfarbstoffen für den Einsatz in tiefer Geothermie.

BSc Chem. Robert Friedrich Steinhoff: On the Photophysical Properties of rGFP in the Gas-phase.

BSc Chem. Sarah Wieghold: Combination of Crossflow Ultrafiltration and Monolithic Affinity Filtration for Concentration of Viruses in Environmental Water.

B.Sc. Theses

Ann-Kathrin Eisenkolb: Auswirkungen der Gasführung von Geothermiebohrungen auf die Reinjektion.

Verena Fink: Developement of a DNA-Microarray for the Quantification of Bacteriophage X174 and Adenovirus 2 in Water.

Leoni Kertess: Optimization of Extraction and Immunological Determination of Eoxynivalenol in Crops

Ulrike Kahl: Optimization of Extraction and Immunological Determination of Fumonisin B1 in Corn and Wheat.

Elena Mraz: Hydraulic Evaluation of a Push-Pull Tracer Test at a Geothermal Well.

Irene Pfeffereder: Catalytic Performance of Alkaline and Earth-alkaline Compounds on Soot Oxidation

Alexander Rinkenburger: Optimization of a Setup for the Enrichment of Diluted Nanoparticle Suspensions by Directional Freezing

Sebastian Weiker: Determination of Reactivity and Kinetics of Diesel Soot by Temperature - Programmed Oxidation and Raman Microscopy

Institute Colloquia

Prof. Dr. Leonhard Ganzer, Clausthal University of Technology, Institute of Petroleum Engineering: Experimental and Numerical Analysis of Polymer Flooding Processes in Oil Reservoirs Using Micromodels (16.1.12)

Prof. Dr. Michel Nielen, RIKILT-Institute of Food Safety, Wageningen, Netherland: Bioaffinity Screening and Mass Spectrometric Identification in Food Analysis (26.1.2012)

Dr. Willem Haasnoot, RIKILT-Institute of Food Safety, Wageningen, Netherland: Experiences with Planar and Suspension Array Immunoassays for Food Contaminants (26.1.2012)

Dr. Stephan Thalhammer und Dipl. Chem. Elisangela Linares, Institut of Radiation Protection, Helmholtz Zentrum München: Online and Retrospective Analysis of the Cellular Microenvironment (27.1.2012)

Dr. Thorsten Schäfer, University of the State of Baden-Württemberg and National Research Center of the Helmholtz Association: The Role of Natural Occurring Nanoparticles on Metal Mobility in the Environment (20.2.2012)

Prof. Dr. Florian Einsiedl, Technical University of Denmark, Department of Environmental Engineering: Life in the Deep, Dark Underground: What Can be Learned from the Molecular Level Perspective (21.2.2012)

PD Dr. Martin Seipenbusch, Karlsruher Institut für Technologie KIT, Institut für Mechanische Verfahrenstechnik und Mechanik: Development of New and Sustainable Materials on the Basis of Function-Optimized Particulate Nanostructures (15.3.2012)

Prof. Dr. Totaro Imasaka, Kyushu University Japan, Graduate School of Engineering, Department of Applied Chemistry: Multiphoton Ionization Mass Spectroscopy Using an Ultrashort Optical Pulse (16.4.2012)

Dr. Katrina Campbell, Queen's University Belfast, Institute of Agri-Food and Land Use: The Rapid Detection of Environmental and Food Biotoxins Using Antibody Based Molecular Interactions Detected Using Planar Waveguide Technology (3.5.2012)

Prof. Dr. Henning Bockhorn, Universität Karlsruhe, Institut für Technische Chemie und Polymerchemie: Flame Generated Carbon Black: Black Magic or Towards Knowledge-based Understanding (6.6.2012)

Dr. Claudia Gärtner, Microfluidic ChipShop GmbH, Jena: Microfluidics -- Technology, Tool Box and Integrated Systems -- From Concept to Routine Use (12.6.2012)

Prof. Dr. Urs von Gunten, Eawag Duebendorf /Switzerland, Department Water Resources and Drinking Water: Oxidation Processes in Water Treatment: Options and Limitations for Micropollutant Elimination (20.6.2012)

Prof. Dr. Frank Keutsch, University of Wisconsin-Madison, Department of Chemistry: Novel Laser-Based Instrumentation: From Kinetics Studies to Global Atmospheric Models (25.6.2012)

Prof. Dr. Lewis Semprini, University Oregon State, School of Chemical, Biological and Environmental Engineering: Silver Nanoparticle Inhibition of the Ammonia Oxidizing Bacterium Nitrosomas Europaea (11.7.2012)

Dr. Stefan Nagl, Institut für Analytische Chemie, Universität Leipzig: Functional Microfluidic Platforms Using Integrated Fluorescent Chemical Sensors (25.7.2012)

Prof. Dr. Werner Nau, Jacobs University Bremen, School of Engineering and Science: Monitoring of Biocatalytic Reactions and Sensing of Analytes with Macrocycles (24.9.2012)

Dr. Oliver Hayden, Siemens AG, Corporate Technology, Erlangen: Using Consumer Electronics to Detect Single Cells in Whole Blood (8.10.2012)

Dr. Carolin Huhn, Forschungszentrum Juelich GmbH: Capillary Electrophoresis Coupled to Mass Spectrometry for the Analysis of Complex Samples (24.10.2012)

Dr. Hans-Heiner Gorris, Universität Regensburg, Institut für Analytische Chemie, Chemo- und Biosensorik: Single Molecule Analysis in Femtoliter Arrays (26.11.2012)

Prof. Dr. Andreas Mandelis, University of Toronto, Institute of Biomaterials and Biomedical Engineering: Thermophotonic and Photoacoustic Methods for Biomedical Measurements and Imaging (27.11.2012)

Dr. Nicole Pamme, University of Hull, Faculty of Science Chemistry: Bioanalysis in Lab-on-a-Chip Employing Magnetic Particles and Cells (6.12.2012)

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

Technical Chemistry (M.Sc.), GIST TUM-Asia

Lecture in Bioengineering & Bioprocessing; Seidel

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 m^3)
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
1 Crossflow-Ultrafiltrationunit (6 m^2-hollow fibre module, Inge-AG)
1 Munich Microorganism Concentrator (MMC 3)
1 Monolithic Affinty Filtration Unit

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

Microarray Technology
2 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 GC/MS, VG Autospec
1 GC/MS, Shimadzu

1 Portable Micro-GC, MITEC
1 Asymmetrical Field-flow-fractionation system, Postnova
2 Concentrators for dynamic headspace analysis
4 HPLC, UV/VIS array detector, programmable fluorescence detector
1 Capillary electrophoresis system
1 Ion chromatograph, Dionex 4500 i
1 Ion chromatograph, Dionex BioLC (Photodiode Array Detector, Electrochemical Detector)
1 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
5 Nd-YAG-laser, pulsed
3 Nd-YAG-laser, cw
1 CO_2-laser
3 Dye-laser (tunable with frequency doubler)
5 N_2-laser
8 Diode-lasers (600-1670 nm; up to 2 W CW)
1 Laser-diode-array with 10 diodes (0.8 µm - 1.8 µm)
1 Laserdiode with external resonator
2 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 UV/VIS spectrometer, analytik jena Spekol 1500
2 Boxcar integrator
4 Digital storage oscilloscopes (400 MHz, 500 MHz)
3 Optical multichannel analysators with monochromators, time-resolving
3 Intensified CCD cameras
2 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 2012

Permanent Staff

Univ.-Prof. Dr. Reinhard Niessner
PD Dr. Thomas Baumann
PD Dr. Christoph Haisch
Dr. Clemens Helmbrecht (-12/12)
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.-Phys. Christoph Berger (6/12-)
Dipl.-Chem. Henrike Bladt
Dipl.-Phys. Benedikt Grob
Dipl.-Ing. Moritz Herbrich
Dipl.-Ing. Gabriele Hörnig (-1/12)
MSc Chem. Maria Hübner (8/12-)
MSc Geol. Wiss. Melanie Kühn
MSc Ing. Hydrogeol. Mark Lafogler
MSc Chem. Veronika Langer (-6/12)
MSc Chem. Sandra Lengger (-9/12)
MSc Chem. Christian Metz
MSc Chem. Susanna Oswald
MSc Chem. Sonja Ott (-5/12)
MSc Pharm. Anal. Lu Pei
MSc Chem. Michael Pschenitza
MSc Chem. Martin Rieger (-1/12)
Dipl.-Chem. Johannes Schmid (-6/12)
Dipl.-Chem. Kathrin Schwarzmeier
MSc Chem. Agathe Szkola (-10/12)
MSc. Chem. Xu Wang (9/12)
MSc Chem. Jan-Christoph Wolf
MSc Chem. Klaus Wutz
MSc Chem. Haibo Zhou

External PhD Students

Dipl.-Phys. Peter Menzenbach (INNOLAS, Krailling)
Dipl.-Ing. Daniel Müller (ABF München)
Dipl.-Biol. Carmen Kocot (Institut Klinische Pathobiochemie München)
Daniela Rascher (HelmholtzZentrum)
MSc Biol. Johannes Otto (DVGW-TZW, Karlsruhe, 11/12)

Diploma Students / Master Students

BSc Chem. Tobias Bauch (10/12)
BSc Chem. Michael Bauhofer (4/12-9/12)
Cand. phys. Christoph Berger (-5/12)
Cand. Chem. Ing. Markus Hager (-5/12)
BSc Chem. Maria Hübner (-6/12)
BSc Chem. Bettina Kiwull (5/12-10/12)
BSc Chem. Fabian Knoller (11/12-)
BSc Geol. Wiss. Bastian Knorr (4/12-9/12)
Bsc Chem. Patrick Kubryck (7/12-)
BSc Chem. Verena Meyer (11/12-)
BSc Geol. Wiss. Elena Mraz (11/12-)
BSc Chem. Anna-Cathrine Neumann (11/12-)
BSc Chem. Edgar Ramon (11/12-)
BSc Chem. Gabriella Somogyi (4/12-9/12)
BSc Chem. Chrysanthos Stergiopoulos (3/12-8/12)
BSc Chem. Sarah Wieghold (3/12-8/12)
BSc Lebensm. Chem. Anika Wunderlich (11/12-)

External Master Students

Ruili Feng (BASF, GIST Singapore, -3/12)
Meera Mahle (BASF, -3/12)
Antonio Meraldo (BASF/GIST, 8/12-)
Clement Ong (BASF/GIST, 7/12-)
Theresa Rock (HelmholtzZentrum münchen, 2/12-6/12)
Robert Steinhoff (HelmholtzZentrum münchen, -2/12)

Guests and Research Fellows

Dr. Ran Li (Oil Crops Research Institute, Chinese Academy of Agricultural, 10/12-11/12)
MSc Nicoleta Elena Mircescu (Babes-Bolyai University Romanian, 9/12-2/13)
Elena Speranskaya (Uni Saratov Russia, 10/11-3/12)
Ilya Voronov (Uni Saratov Russia, 10/11-3/12)
MSc Danting Yang (Uni China, 9/12-9/13)

Student Assistants

Ann-Kathrin Eisenkolb (7/12-8/12)
Ronja Kuhne (2/12-5/12)