Annual Report

Institute of Hydrochemistry

Chair for Analytical Chemistry

2009

Institute of Hydrochemistry
Chair for Analytical Chemistry
Technische Universität München
Marchioninistr. 17

D–81377 München

http://www.ws.chemie.tu-muenchen.de

Editor: Dr. Thomas Baumann

Editorial

Dear coworkers, friends and colleagues,

despite the expectations we had at the beginning of 2009 the Institute of Water Chemistry (IWC) is still on track for being a successful research unit.

First of all, in Spring 2009 the institute was again flooded by Bachelor and Masters Students doing their experiments at the IWC. Although this is an acknowledgment of an interesting research program and excellent supervision; a total of 21 BSc and 11 MSc theses is quite something to read during cold winter days. The number of finished PhD examinations peaked: 9 PhD candidates graduated, two of them with summa cum laude.

The theses reflect the broad research spectrum which is unique for the IWC: micro array reader development, antibody production and validation, diesel soot characterization, particle separation by laser photons, geothermal well characterization, groundwater protection and site remediation, bio film inspection in micro channels, synthesis of molecular imprinted polymers, development of enrichment procedures for bacteria & viruses, studying engine heat-exchanger blocking, ...

How can one be successful with such diverse topics? The answer is simple: by establishing excellent working groups which are jointly developing new measurement technologies and new applications. As the King of Prussia said (Königgrätz, 1866): "Move separately, strike united". Well, and asked for the difference between a physicochemist and an analyst, my answer is: we're not limited to one matrix.

Last year we received funding of 1.2 million EUR covering the whole diversity of the research groups. Not too bad within the economic crisis. Thanks to our "Circle of Friends" we were again able to spend some start-up money on research ideas.

Through intense work of various group leaders we got funded some new equipment: Orbitrap MS, Biacore SPR reader, and a second High-tech Raman microscope.

There is still a lot to do. Since 20 years I'm now appointed chair of Analytical Chemistry, and most of the equipment (and we possess a lot...) needs to become renewed. So, within the next years besides exciting research topics we will have to focus on this, too.

All the best for the year 2010!

Reinhard Niessner
Head of the Institute

Head of the Institute and Group Leaders 2009

C. Helmbrecht, R.Nießner, T. Baumann, D. Knopp, C. Haisch, M. Seidel

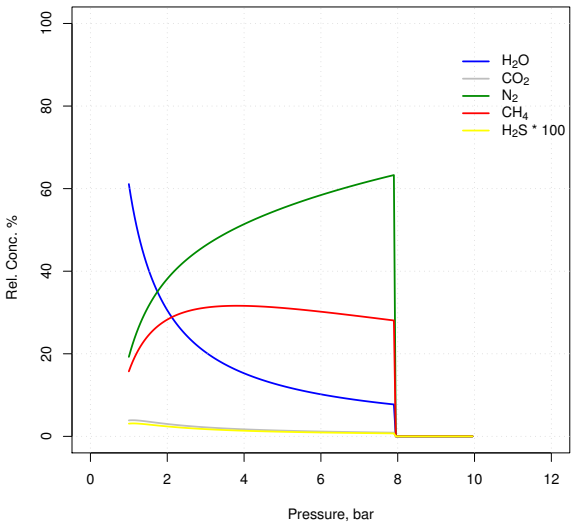
1 Research

1.1 Hydrogeology and Hydrochemistry (Head: PD Dr. T. Baumann)

1.1.1 Gas Composition and Hydrogeochemistry of the Malm Aquifer

Funding: BMU (Federal Ministry for the Environment)
Cooperation: FU Berlin; GGA Hannover; LfU Bayern; Erdwerk GmbH, München; HydroConsult GmbH, Augsburg

The Malm aquifer is one of the most important deep groundwater aquifers in the Bavarian Molasse Basin. Especially around Munich several new projects for geothermal exploration have been realized. Detailed knowledge of the hydrochemical character of the thermal water as well as the hydrogeochemical processes in the aquifer is a prerequisite for the design of the geothermal power plant. Our research is focused on the processes, which are relevant for the stability and security of the geothermal well. One of these processes is the occurrence of a free gas phase with critical gases like H_2S. With isotopic measurements on thermal water it was possible to study the genesis of H_2S in the Malm aquifer. At numerous wells water samples were taken to analyze the isotope ratios of ^{34}S in hydrogen sulfide and sulfate. The results show an enrichment of the heavier isotopes which suggests the production of H_2S by thermophilic reduction of sulfate in the presence of methane. An impregnation of the thermal water with sour gas can be ruled out.



Constituents of the gas phase of the groundwaters in the Malm aquifer

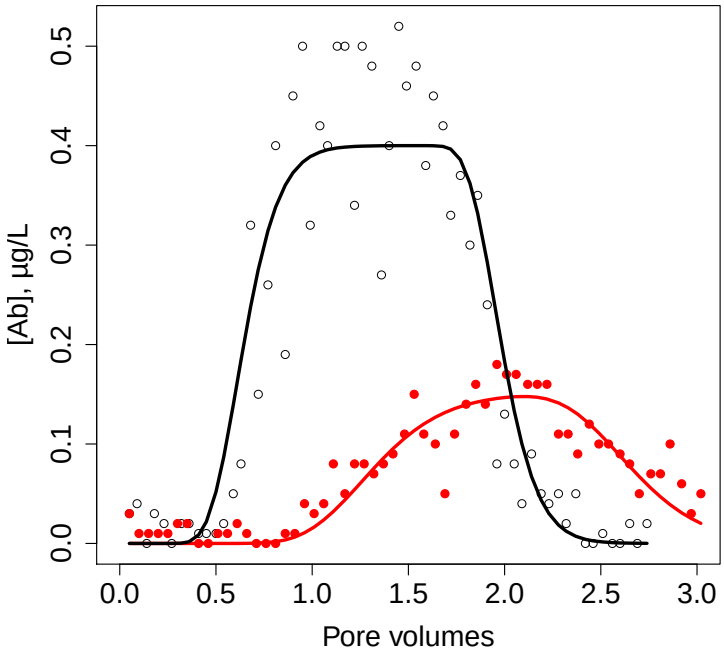
Another point of interest is the degassing process in the geothermal well. For the optimal establishment of a geothermal power plant it is important to avoid a free gas phase in the construction. Free gas could lead to a lower heat transfer, the precipitation of minerals within the heat exchanger, and increased corrosion rates. Therefore calculations were made to determine the degassing pressure. The figure shows an hypothetical example of the degassing pressures and the gas composition. First gas bubbles are built at 8 bar, where the solubility for nitrogen is exceeded. From this point all dissolved gases equilibrate with the gas phase according to their partial pressure and the Henry constants. With increasing gas volume the relative proportion of CO_2, N_2, CH_4 and H_2S decreases, because the transfer is mass limited.

A detailed investigation of the corrosion processes will be included into the hydrochemical research program. To get information about scaling processes and corrosion, test materials will be installed into the bypass loop of a geothermal facility and later analyzed by SEM/EDX.
(*C. Mayr*)

1.1.2 Visualization and Quantification of Processes at Biogeochemical Interfaces with Magnetic Resonance Imaging

Funding: DFG (German Research Foundation)
Cooperation: Partners in the Priority Program SPP1315

Biogeochemical interfaces in soil are important for the retardation and degradation of pollutants. The interfaces vary in the spatial and temporal domain and access to the interfaces is controlled by the topology of the pore space. Magnetic resonance imaging (MRI) is a powerful technique for noninvasive visualization of porous systems and contaminant transport. However, the sensitivity of MRI for trace concentrations of contaminants is limited and only few contaminants can be visualized directly. MRI tracers have the potential to overcome this deficiency.



Breakthrough curves of anti-BaP antibodies through silica gel w/ and w/o BaP-coating

During the first part of this project anti-B[a]P antibody-labeled nanoparticles were synthesized and tested in different column setups. Magnetic nanoparticles were produced by alkaline precipitation of iron oxide and have a size between 60 and 300 nm. Monoclonal anti-B[a]P antibodies were coupled to the iron oxide nanoparticles. While magnetic nanoparticles decrease the MRI signal, similar nanoparticles with a gadolinium oxide core will enhance the MRI signal.

Due to the size of the nanoparticles, not all of the pore spaces and interfaces in a system are accessible to the MRI tracer. What seems to be a design flaw can turn into an advantage, because the nanoparticles will gain access only to interfaces which are accessible to bacteria as well. In contrast to dissolved tracers a selective visualization of interfaces becomes possible.

The breakthrough curves of the antibodies through silica gel suggest that the antibodies bind to B[a]P, but only if B[a]P is coupled to the silica gel through a spacer molecule. B[a]P is not detected if adsorbed flat to the surface. The spacer was introduced by silanization of the silica gel with aminopropyltriethoxysilane (APTES). Then, a carboxy modified B[a]P (B[a]P-1-butyric acid) was coupled covalently to the amino group.
(*M. Rieger*)

1.1.3 Nanoparticles at the Interface between Atmosphere and Hydrosphere

Funding: Gottlieb Daimler- and Carl Benz Foundation

Nanotechnology is considered as the key technology of the 21th century due to the specific material characteristics of nanomaterials and nanostructured materials. This advance enables the development of new products in all industrial sections. The business volume in 2007 was about 52 billion $ worldwide.

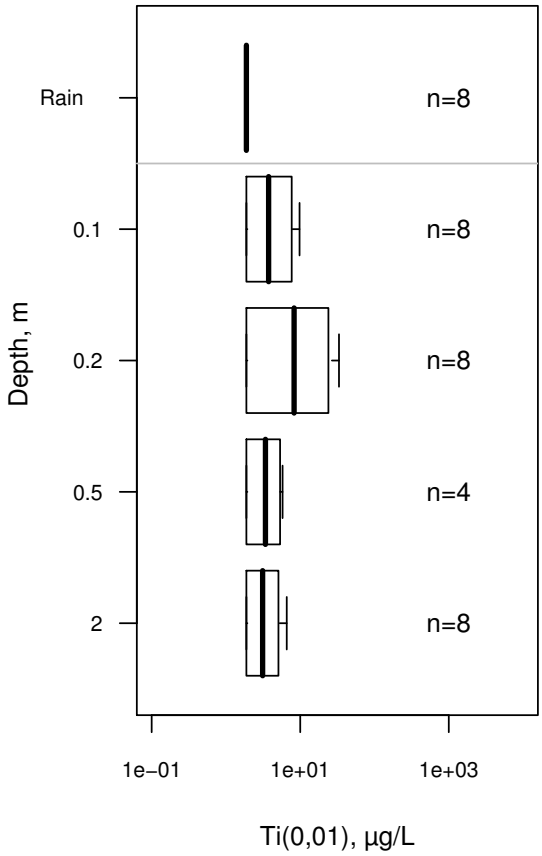
Despite of their commercial success, the benefits of synthetic nanomaterials might disguise potential environmental risks. For example, weathering processes cause a release of nanomaterials from construction materials, into the environment. A likely pathway is airborne transport and deposition on the ground surface together with precipitation or as dry deposition (dust).

The field laboratory of the Institute of Hydrochemistry enables to pursuit the immission of synthetic nanoparticles at the interface between atmosphere and hydrosphere and the transport through the unsaturated zone to the ground water of a glacial sand and gravel aquifer. Samples of the seepage water were taken regularly in 9 layers in the unsaturated zone. In combination with the wet-only/dry-only samplers the transport of the nanoparticles can be quantified. The concentrations of the inorganic substances in the different size ranges were separated by ultrafiltration and asymmetrical flow field-flow fractionation (AF4). Analysis will is done by SEM/EDX, Raman microscopy, and AF4/ICP-MS.

The results of the monitoring in 2009 reflect the environmental setting of the field laboratory. The distribution of the inorganic substances varies with particle size and depth. Most of the measured elements showed a maximal concentration in January and February during heavy rain fall or melting snow. This is when the preferential pathways are open and a release of particles occurs in all depths. The titanium concentration in the particle fraction from 10 - 100 nm in March 2009 is plotted in the figure for the upper part of the vadose zone. The lowest titanium concentrations were measured in rain water with 1.9 μg/L and increases in the subsoil to 8.3 $\pm$25 μg/L (0.2 m).

Long term measurements under natural conditions are necessary for a sound assessment of the transport properties of synthetic nanoparticles. The monitoring at the Munich well will be complemented by tracer tests.

(*S. Huckele*)



Distribution of nanoparticulate Ti in the unsaturated zone

1.1.4 Application of a Strategy to Decrease Well Aging at a Multiple Contaminated Site

Funding: Mitteldeutsche Sanierungs- und Entsorgungs GmbH

The Bitterfeld-Wolfen area is known for lignite mining and its chemical industry, but also for its contaminations of groundwater and soil. There are about 5000 contamination sites spread over an area of 10 km^2. These contaminations are far too complex to be treated individually.

As a consequence, the entire area is treated in the framework of a ecological super project. There are numerous groundwater wells to ensure an appropriate groundwater level in the city of Bitterfeld and to prevent the propagation of contaminants into the surroundings. Recent investigations show a massive decrease of the specific yield in some of those wells, due to incrustations and precipitation of organic matter at the well screens, pumps, and draining pipes. The incrustations impair the proper operation of the wells and also increase the costs for the hydraulic barrier.

CO_2-treatment of a groundwater well

It had been shown previously that the augmentation of water enriched with carbon dioxide into the pumping cone of a can inhibit incrustations and precipitation and thus help to maintain proper operation of the wells. The technique of CO_2 augmentation was therefore adapted to another hydraulic barrier.

The installation of the hydraulic barrier was accompanied by a depth-resolved hydrochemical screening and the individual wells were carefully adjusted to the local hydrogeological and hydrochemical conditions. The augmentation with CO_2 was adjusted to reach a pH below 8.3 at a minimum injection rate.

The behavior of the augmented well over a duration of 6 months showed no permanent decrease of the specific yield. However, the water levels at the entire hydraulic barrier did decrease sharply. This suggests a local aquifer boundary.

Due to the high concentration of organic solvents in the groundwater flocculation of the organic carbon, as observed in the previous study, was suppressed. However, the pumps and pipes of the well with CO_2 augmentation were in a better shape compared to those without CO_2 injection.

(*T. Baumann*)

1.2 Bioanalytics (Head: Prof. Dr. D. Knopp)

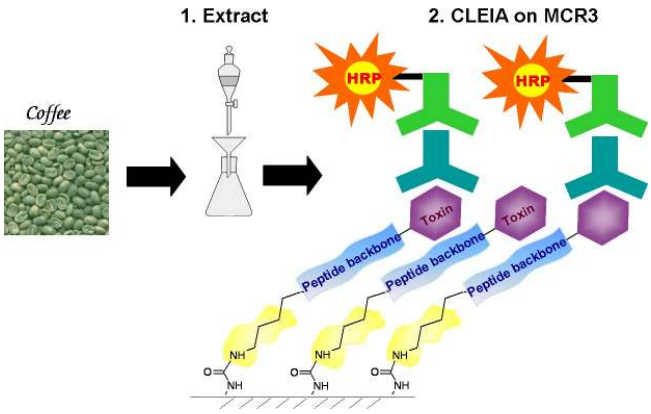
1.2.1 Hapten Microarray-based Screening of Mycotoxins in Food Samples

Funding: BMBF (Federal Ministry for Education and Research)
Cooperation: Eurofins Analytik GmbH; Wiertz-Eggert-Jörissen, Hamburg; Ring Engineering Ltd., Azur, Israel

Mycotoxins, even when present in low concentrations, represent a potential hazard to human health and more than 90 countries worldwide have directed considerable efforts to introduce, regulate and standardize the levels of mycotoxins in food and animal feed.

In particular, ochratoxin A (OTA) is a mycotoxin known to cause nephrotoxicity and nephrocarcinogenicity when ingested by human beings and animals. OTA is produced as a secondary metabolite by fungi from the genus Aspergillus and Penicillium versucosum and it is most commonly found as a contaminant of wheat and wheat products, but can also contaminate dried fruits such as figs and raisins, green coffee and coffee products, beer, wine, cocoa and even meat.

The most widespread analytical procedure for the detection and quantification of OTA in several food commodities usually consists of HPLC/UV-Vis, and/or mass spectrometry. Immunoaffinity clean-up (IAC) has been widely developed and turned up for several foodstuffs as a powerful pre-treatment method for HPLC.



Schematic representation of the Ochratoxin A analysis of green coffee samples

The enzyme-linked immunosorbent assays (ELISA) are a viable alternative to the most sophisticated HPLC-based procedures, since the food extracts can be analyzed with little or no pre-treatment. Therefore, in this project, the previously developed Munich Chip Reader 3 and namely developed biochips are tested for the determination of mycotoxins. While in the past main focus was devoted to aflatoxins, the determination of OTA in green coffee with as little pre-treatment as possible was the main aim of the previous period. In particular, a peptide-derivatized OTA was covalently immobilized on a chemically modified glass chip and used as the solid support for a flow-through indirect competitive ELISA. The results are promising: after calibration of the equipment one individual sample determination takes 12 minutes. The same chip is used and regenerated along the calibration process and the measurement of the unknown sample and the number of regeneration cycles that it can undergo is 20, allowing for calibration with 8 standards and measurement of 6 unknowns. The detection principle is chemiluminescence which is performed by means of a CCD camera.
(*J. Sauceda-Friebe*)

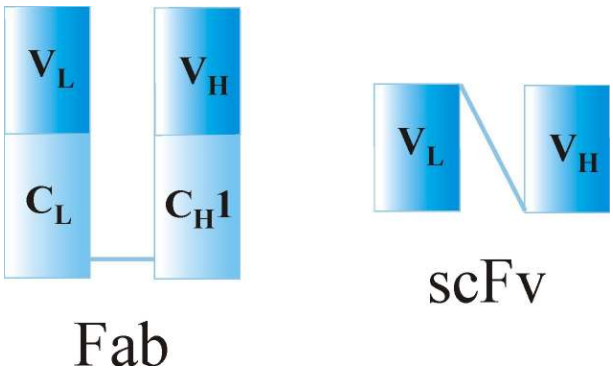
1.2.2 Recombinant Antibodies Against the Polycylic Aromatic Hydrocarbon Benzo[a]pyrene

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

Polycyclic aromatic hydrocarbons (PAHs) are formed as a result of incomplete combustion of organic compounds. In the European Council Directive 98/83/EC concerning the quality of water intended for human consumption (drinking water directive) a limit value of 10 ppt was set for benzo[a]pyrene (B[a]P) which is the lowest of all threshold levels set for individual chemical parameters in this directive.

Sensitive and reliable analytical methods are needed to evaluate the presence of B[a]P at very low concentration in several matrices. In the past, we reported on the development of a highly sensitive indirect competitive ELISA for the detection of B[a]P in potable water. Fourteen monoclonal antibodies were generated in mice using novel B[a]P derivatives. With the best antibody (clone 22F12) an LOD of 24 ppt was obtained. From the 16 EPA-designated PAHs, only chrysene, indeno[1,2,3-cd]pyrene, and benzo[b]fluoranthene showed a cross-reactivity (CR) higher than 20%. No CR was observed for two- and three-ring PAHs as well as dibenz[ah]anthracene and benzo[ghi]perylene.

In this new project, the properties of B[a]P antibodies will be further optimized using genetic engineering. Antibody genes can be amplified by PCR and expressed in different expression systems in various formats, such as the Fab, Fv, and single chain Fv (scFv). The major advantage of these antibody fragments is that they are smaller in size and therefore easier to manipulate genetically and express in bacterial systems. Up to the present, recombinant antibodies were prepared for only a few environmental chemicals, mainly pesticides. The recombinant antibodies prepared in this project, will initially be tested using surface plasmon resonance on specially prepared chips and newly synthesized PAH-derivative conjugates. Further, the effect of pH value, ionic strength, and inorganic ions on both signal and sensitivity of the ELISA will be studied. Beside further increase of antibody affinity also specificity should be tuned to meet the required specificities.
(*X.Y.Z. Karsunke*)



Schematic drawing of scFv and Fab fragments.

1.2.3 Bioanalytical Applications of Biofunctionalized Nanoparticles

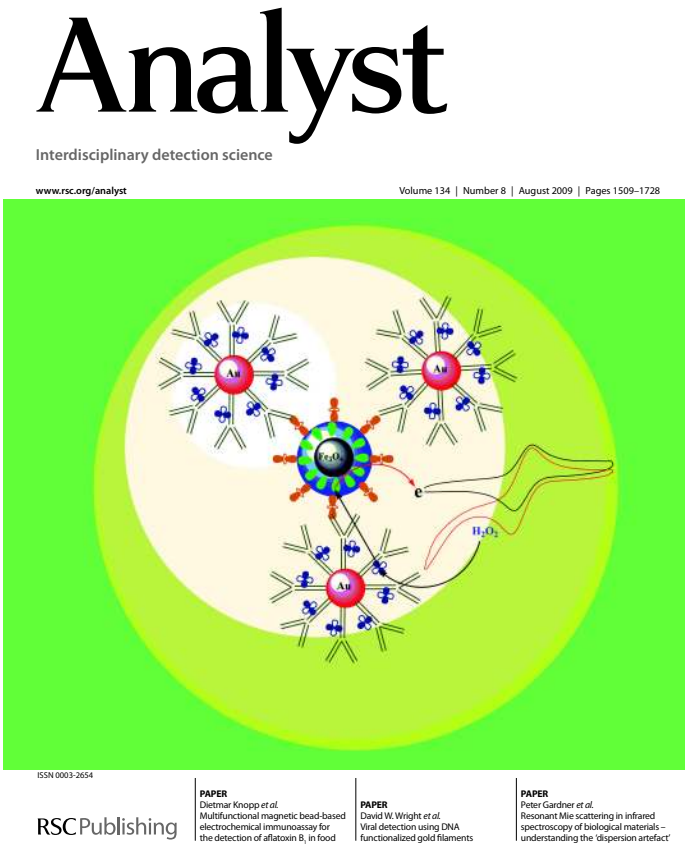
Funding: Alexander von Humboldt-Foundation

The emerging research field of nanotechnology, the process to generate and manipulate nanomaterials, provides excitingly new possibilities for advanced development of new analytical tools for bioanalytical applications. In addition, the conjugation of different moieties to the nanoparticles (NP) widens their application fields. Despite achievements in the fields of label-free bioassays, labeling techniques will continue to play a leading role in this area. Importantly, NP offer elegant ways of interfacing biomolecule recognition with inherent signal amplification.

Our research has looked to develop powerful biofunctionalized nanometer-sized silica particles. The silica shells of these particles facilitate a variety of surface reactions and allow conjugation with biomolecules. They are an ideal protein host since they are highly chemically and thermally stable, they have a large surface area, and exhibit a fine dispersibility in aqueous solution. Furthermore, silica NP are optically transparent.

A variety of NP consisting predominantly of a silica shell and various encapsulated molecular tags for use in advanced bioanalytical detection was synthesized, e.g. multifunctional magnetic beads, core-shell SiO_2/Au nanocomposites, and rhodamine doped silica nanoparticles. The biomolecules used for conjugation to the NP were target analyte-protein conjugates (aflatoxin B_1-bovine serum albumin, AFB_1-BSA; BSA; antibodies (anti-aflatoxin; anti-IgG) or enzymes (horseradish peroxidase, HRP, glucose oxidase, Gox). Independent of the detection principle such as electrochemical detection (highly sensitive and reusable electrochemical immunoassay for AFB_1 in food samples), fluorescence detection (fluorescence immunoassay for AFB_1 in food samples using AFB_1-BSA-modified magnetic core-shell silica NP and anti-AFB_1-functionalized rhodamine B-doped silica NP) and visible inspection (NP-based lateral-flow immunodipstick using magnetic nanogold microspheres with nano-Fe_2O_3 particles as core and gold NP as shell which are biofunctionalized with anti-AFB_1 antibodies) a moderate increase in sensitivity compared to conventional assays was obtained.

(*D. Tang*)

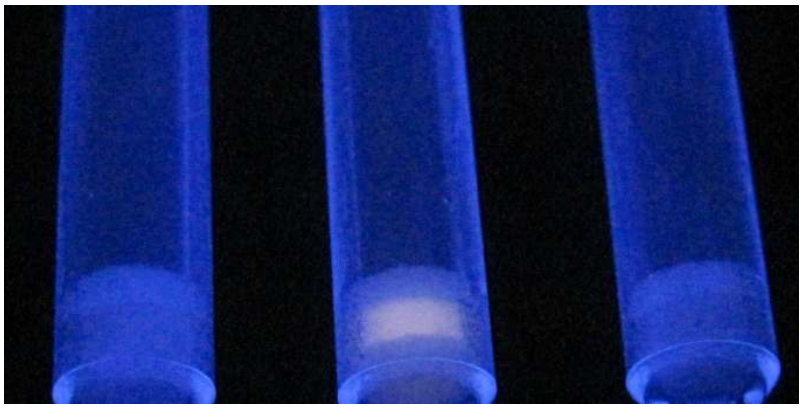


The multifunctional magnetic bead-based immunoassay made it to the front page of Analyst (134, 2009, 1509)

1.2.4 Development of Immunochemical Tests for Rapid On-site Screening

Funding: DAAD (German Academic Exchange Service)
Cooperation: Department of Common and Inorganic Chemistry, Chemistry Faculty, Saratov State University, Saratov, Russia

The increasing number of environmental and food contaminants and continuous lowering of set limit values calls for fast, cost-effective, high-sensitive analytical techniques for on-site screening. In the last decade, beside miniaturization and ruggedization of conventional instrumentation to permit its use in a field setting, new technologies have been developed for field monitoring purposes. Originating from clinical chemistry, these technologies, first of all lateral-flow immunochromatographic strips, were adapted to solve food control and safety problems. However, only a few attempts were undertaken for spreading such tests for the screening of low-molecular weight contaminants in environmental and food samples. The limited sensitivity of corresponding tests can be considered as the main obstacle for further propagation.



Gel-based immunoassay using quantum dots as label. Left: control (without B[a]P antibody); middle: blank (no B[a]P in sample); right: 5 ng B[a]P in sample.

In a previous project, a gel-based immunoassay, performed in test columns (Bond Elut cartridges), was developed for highly sensitive and reliable detection of Benzo[a]pyrene (B[a]P) in water samples. It combines preconcentration and detection of the target analyte using anti-PAH antibodies and horseradish peroxidase-B[a]P tracer conjugate in one single cartridge. The preconcentration is based on immunoaffinity extraction, i.e., trapping of the target analyte(s) by antibodies immobilized on a column and washing off extraneous compounds before detection.

In a follow-up project, a new approach was started, which combines immunoaffinity preconcentration with competitive immunoassay principle and sensitive detection and read-out by a hand-held reader system. Main emphasis was put on the examination of selected labels, both newly synthesized and commercially available ones, for example, enzymatic label, gold nanoparticles and quantum dots (QDs). B[a]P was used as model analyte. Finally, with the most promising label the rapid on-site test will be developed. (*I.Yu. Goryacheva, N. Beloglazova, A. Proydakova*)

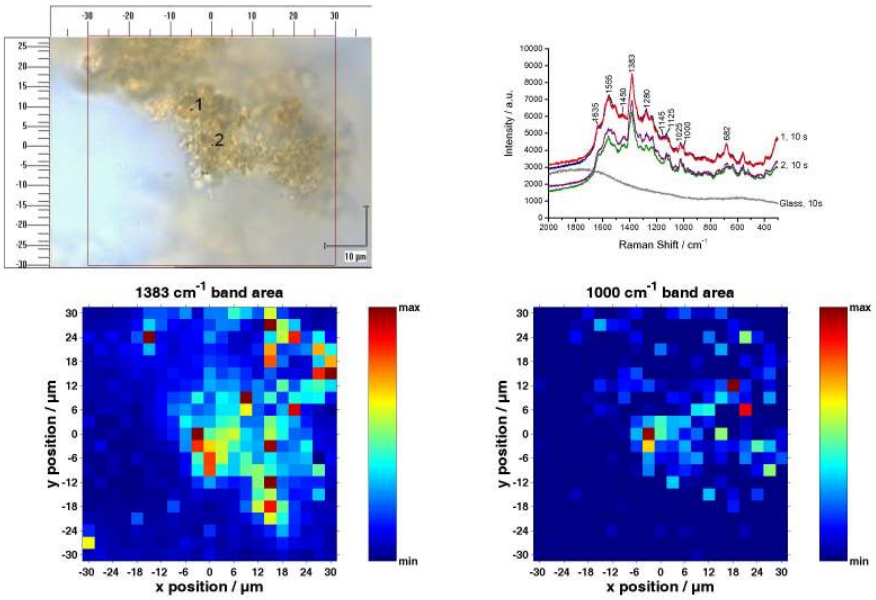
1.3 Applied Laser Spectroscopy (Head: Dr. C. Haisch)

1.3.1 Raman Microscopy and Surface-Enhanced Raman Scattering (SERS) for In-Situ Chemical Analysis of Biofilm Matrix

Funding: DFG
Cooperation: Prof. Horn, TUM

Biofilms are interface-associated communities of microorganisms embedded in a matrix of extracellular polymeric substances (EPS, such as polysaccharides, proteins, glycoproteins, nucleic acids, lipids, and humic-like substances). Biofilms represent a prevalent mode of microbial life on Earth and can be found on nearly all interfaces (solid–liquid, solid–air, liquid–liquid, and liquid–air). Therefore, detailed information about chemical composition and structure of the biofilm matrix is of great importance for different fields (in particular, for medical and technological processes).

Raman microscopy (RM) is a nondestructive analytical technique which is based on the effect of inelastic light scattering by molecules. RM is a capable tool which provides whole-organism fingerprints for biological samples with spatial resolution in µm range. Low water background makes RM beneficial for in situ studies of biofilms, since water is the major component of the biofilm matrix. We apply RM for chemical characterization of different structures in a multispecies heterotrophic biofilm matrix, including microbial constituents and EPS. Information about the distribution of different components in complex biofilm matrix can be obtained by Raman mapping. In this case the spectra from distinct biofilm area are obtained step by step. The subsequent band analysis for collected spectra allows us to create the corresponding maps or chemical images of biofilm. However, Raman mapping is very time consuming (at least 10 s is required for each single spectrum), the obtained Raman spectra contain only a few bands and therefore rather limited chemical information is available.



Microscopic image, Raman spectra and spectral mapping of biofilm

We show that enhancing the sensitivity of RM by surface-enhanced Raman scattering (SERS) allows for much faster biofilm analysis. The SERS effect takes place when the analyte molecules are attached to, or in the immediate proximity, of metallic (Ag, Au, or Cu) substrate with nanometer-roughened surface. The total enhancement factor due to electromagnetic (localized surface plasmon resonance) and chemical (charge transfer) enhancement is in the range of 10^3 - 10^6. In some cases (at hot spots – closely

spaced particles or rough nanostructures) signal enhancement up to $\approx 10^{14}$ can be achieved. We employ colloidal silver nanoparticles for in situ SERS measurements of biofilm by RM and obtained reproducible SERS spectra from different biofilm constituents. The achieved enhancement factor of several orders of magnitude along with the resolved issue of SERS reproducibility enable us rapid (about 1 s for a single spectrum) SERS mapping or chemical imaging of biofilms. The figure illustrates microscopic image of biofilm as well as corresponding SERS spectra and SERS maps for bands at $1383\,\mathrm{cm}^{-1}$ (sym COO^- str vibrations, characteristic for polyanionic polysaccharides) and at $1000\,\mathrm{cm}^{-1}$ (Phe ring breath, typical for proteins).

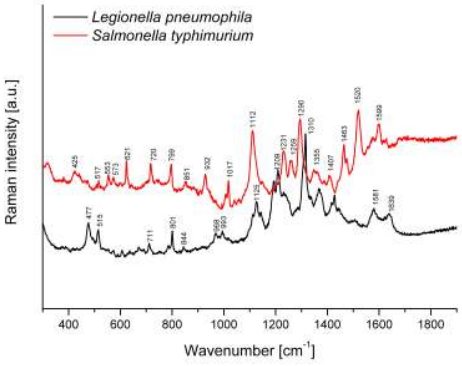
Thus, RM in combination with SERS can be an efficient tool for sensitive chemical in situ analysis of biofilms, including the detection of different components and the determination of their relative abundance in the complex biofilm matrix even at low biomass concentration.
(*N. P. Ivleva*)

1.3.2 Label-Free In-Situ Microarray Detection of Microorganisms in Water Based on Surface-Enhanced Raman Scattering

Funding: IWC

Surface-enhanced Raman scattering enables enhancement of low Raman scattering and allows obtaining fingerprint spectra of different biological systems even to the single molecule level.

A variety of metal structures (Ag, Au and Cu) is used to induce the SERS effect. We have studied the suitability of different Ag colloid sols as SERS substrates for the analysis of microorganisms. Additionally, we have developed a label-free in situ detection principle of microorganisms on a microarray chip using SERS. The total assay time of the method is 65 minutes and requires a total reactant volume of 28 mL to analyze cells in an aqueous environment. Thus, our method offers the advantages of reduced assay times, simple handling and lower reactant volumes compared to methods where the target molecules need to be labeled. We have prepared stable, monodispersed silver colloid sols in a reproducible way by reducing silver nitrate with hydroxyl amine hydrochloride, according to a modified procedure of Leopold and Lendl. These colloids show a long shelf life and their implementation for SERS is successful. We have investigated the effect of their agglomeration rates on the increase of SERS cross section of Crystal Violet. Three different bacteria, two heat-killed (L. pneumophila and S. typhimurium) and one living (E. coli) species, in aqueous environment have been detected in situ and show clearly distinct fingerprint spectra with high SNRs. An optimized incubation solution of the analytes has been found, which enables direct Ag particle agglomeration towards the cell wall, hence increases the number of particles surrounding the analyte during detection.



Fingerprint spectrum of L. pneumophila (black) and S. typhimurium (red). Their amide III band at $1290\,\mathrm{cm}^{-1}$ and $1310\,\mathrm{cm}^{-1}$ respectively, were used for SERS mapping

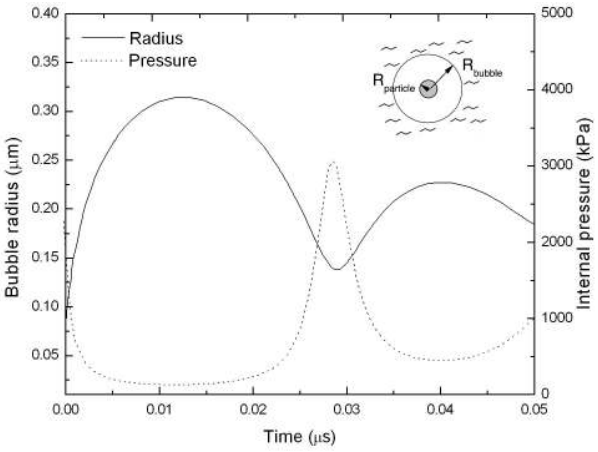
This results in hot spots which again results in improved sensitivity. We have been able to develop calibration curves through Raman mapping of both L. pneumophila and S. typhimurium (see Figure). An assignment of the Raman bands has been carried out for both species. Our preliminary results indicate a good perspective for the adoption

of SERS for microorganism characterization. As the detection is carried out in aqueous environment, a non-destructive analysis is possible. The synthesized particles can also be used for a variety of other SERS applications. The method can provide us with new information about the binding between antigen and antibody in the future, which again can give us a better knowledge on biological activities in microorganisms. To further optimize the method, in vitro agglomeration of the SERS substrates will be carried out in the future. By this method, the particles can be immobilized on specific sites, rich in N and S functional groups, for different recognition purposes. Integration in an automatic fluidic system is also in preparation.
(*M. Knauer*)

1.3.3 Laser Induced Nano-bubbles on Functionalized Nanoparticles

Funding: DAAD, Facultad de Ingeniería, Universidad de Buenos Aires (FIUBA); China Scholarship Council (CSC)

Metal nanoparticles with strong plasmon resonance absorption, tunable in the visible and near-infrared spectral ranges, present additional benefits for photoacoustic (PA) detection. Laser interactions with suspensions of nanoparticles (NPs) in aqueous media have been extensively studied with the goal to develop biosensors, medical imaging and therapeutic applications. Sensitivity for biosensors, cell and tissue imaging systems based on strongly absorbing metal (gold and silver) NPs can be achieved by laser PA. We look into the application of PA effect by laser-induced nanobubbles (LINB) on colloidal gold solutions with different nanoparticle sizes. Under certain conditions, theoretical and experimental results show that the PA signal generated by LINB is not proportional to the absorption, but it is strongly related to the size of gold NP (GNP) in aqueous solution. Moreover, this kind of PA configuration has a great potential to detect and quantify biomolecules. Currently, we are studying its application in biomolecules based on GNP aggregation. Since the aggregation can be understood as a particle size change process, this PA system could be more sensitive than other conventional spectroscopy methods.
(*M. Gonzalez, Xiangjiang Liu*)



Bubble radius and pressure transients of the water vapor inside the bubbles as calculated from the Rayleigh-Plesset equation. The first maximum in pressure at 29 ns marks the collapse of the bubble; the following modulations are only expected for oscillatory bubble motion

1.3.4 Synthesis of Core-Shell Surface-Enhanced Raman Tags for Bioimaging

Funding: DAAD, China Scholarship Council (CSC); Facultad de Ingeniería; Universidad de Buenos Aires (FIUBA)

We present a rapid and straightforward procedure for the synthesis of core-shell surface-enhanced Raman scattering tags. SERS tags are combinations of Raman active dyes with metallic nanoparticles inducing the enhancement. Because of their significantly higher stability to environmental conditions, the majority of SERS tags are designed in core-shell geometry. The main disadvantage of this approach up to now was the time-consuming (normally days) and complex preparation of these labeled core-shell particles. The presented approach can be performed within hours on

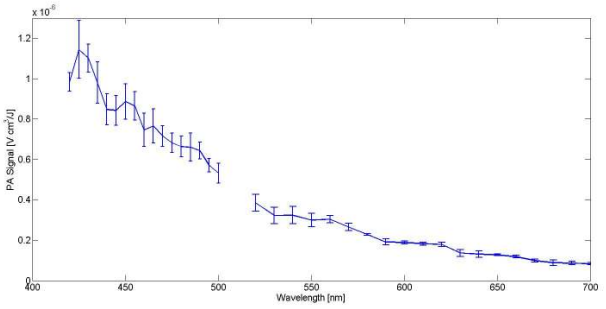
a daily base. The main characteristics and the stability of the fabricated SERS tags in extreme pH values, high ion strength, or in organic solvent is demonstrated in this communication. Furthermore, the SERS tags are functionalized with anti-Salmonella antibody as a model to present a potential application of the core-shell particles in bioimaging.
(*Xiangjiang Liu, M. Gonzalez*)

1.3.5 New Pulsed Photoacoustic Aerosol Spectrometer

Funding: IWC

The photoacoustic (PA) process is based on a light–matter interaction. The absorbed photon energy is transformed into a local heating followed by an expansion resulting in the generation of a sound wave. Usually modulated continuous wave (cw) light, generated by laser diodes, is used as a light source. The disadvantage of this method is the limited number of available wavelengths and the very narrow tuning range defined by the laser diode technology.

In our new spectrometer we use a flash-lamp pumped Q-switched Nd:YAG laser as the light source. This kind of laser is generating short light pulses in the range of 5 ns with intensities beyond 200 MW/cm^2 allowing high efficient non linear processes. In this case the third harmonic (355 nm) of the Nd:YAG laser is pumping a Optical Parametrical Oscillator (OPO). These OPO systems are generating two beams, the signal beam with a tuning range of 410 - 710 nm and the idler beam with a tuning rage of 710 - 2600 nm, simultaneously. These two beams and a part of the 355-nm beam are passed through three PA cells. Pinholes are placed before the PA cells allowing the reduction of the beam diameters. Finally, the beams are dumped by pyroelectric detectors responsible for the pulse energy measurement of each individual pulse.



Absorption spectrum of sparc-generated soot, measured with the new instrument

Inside the PA cells a microphone is detecting the acoustic signal generated by aerosol particles pumped through the PA cells. The amplified microphone signals are stored and analyzed in a data acquisition system. The new spectrometer was successfully tested by measuring the PA spectrum of different classes of aerosol particles like polystyrene, soot and lycopodium. The spectrometer reaches a resolution better than 10^{-4}cm^{-1}.
(*P. Menzenbach*)

1.4 Laser-based Separation (Head: Dr. C. Helmbrecht)

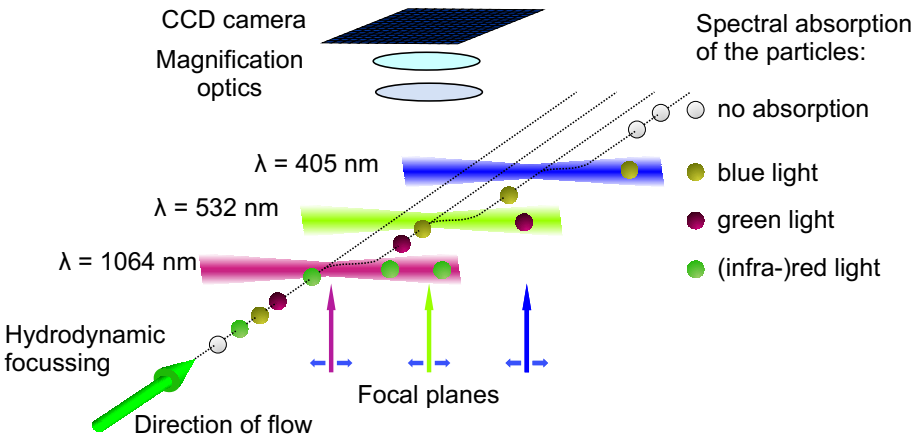
1.4.1 Online Characterization of Irregularly Shaped and Absorbing Particles by Photophoresis

Funding: DFG

A large number of techniques for the analysis of particles mainly focus on the parameter particle size. With the application of light the optical properties of the particles such as refractive index and absorption become accessible. Due to exchange of momentum between photons and matter forces are generated. In case of a strong light source, e.g. laser, and sufficient small masses, e.g. microparticles, forces induced by light become capable of manipulation and trapping of particles. The migration induced by light is termed photophoresis (PP).

The application of optical forces on particles suspended in liquids is a new approach for characterization and separation of colloid matter. As the PP migration is directly linked to the intrinsic properties of the particles, the particle velocity is a function of radius and refractive index and absorption. Hence, the evaluation of particle velocity (Photophoretic Velocimetry) is of great value for the determination of radius and refractive index of single particles.

Besides ideal spherical and monodispersed samples the analysis of irregularly shaped and absorbing particles is of interest for the characterization of real world samples as the majority of particles is polydispersed and not spherical. For the characterization of particles a set-up is currently under development. The figure shows the principle of the set-up. Laser beams are focused in the flow cell. By using different wavelengths, the influence of absorption on the migration behavior can be studied. Spherical particles in the proximity of the beam are centered in the beam and start migrating in the direction of the beam propagation. An automatic routine for image processing determines the particle velocities.



Schematic of photophoretic characterization

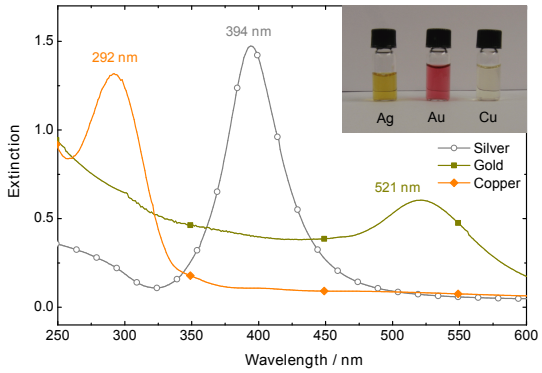
In that way, particles with different sizes or refractive indices can be discriminated. Techniques on the basis of light induced forces are excellent techniques for contact-free sample handling with high resolution characterization and separation of particles, cells and bacteria.

(*C. Helmbrecht*)

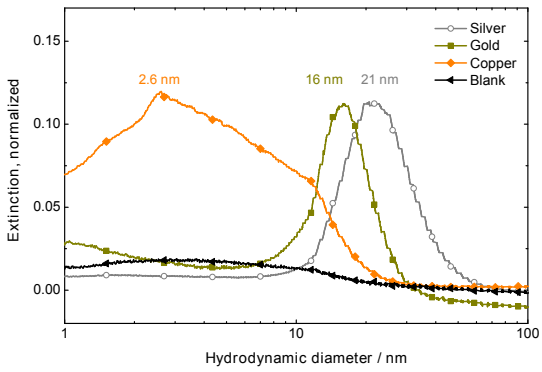
1.4.2 Evaluation of Nanometer-sized Metallic Particles in Water Suspensions Using Asymmetrical Flow Field-Flow Fractionation and Inductively Coupled Plasma Mass Spectrometry (AF4-ICPMS)

Funding: IWC

The possibility to tune the properties of metallic nanoparticles is utilized in spectroscopy, biochemistry, catalysis and medicine. Gold particles are frequently used as location markers in studies of biological specimen. Silver sols serve as optical absorbers with tailored optical absorption properties, making other sols of other metals such as gold or copper particles highly favored substrates for surface-enhanced Raman scattering spectroscopy (SERS). The hyphenation of AF4 and ICPMS enables the determination of abundance of elements related to particle size directly in aqueous samples.



Particle size distribution by asymmetrical flow field-flow fractionation



Optical absorption spectra of Cu, Ag and Au sols by UV/Vis spectroscopy

As the particle properties are strongly related to size, a precise determination of absolute size as well as particle size distribution is of great importance to verify stable conditions of particle synthesis. In addition, metal sols are sensitive to temperature, light and the presence of ions in the solvent and may alter rapidly their size. For that reason, the stability of metallic sols was systematically evaluated in order to obtain reproducible particle size.

Electron microscopy (EM) is an excellent technique to derive particle size distributions. However, as particles are deposited on a filter prior to analysis, this is a very time consuming method. Since the analysis in EM takes place under vacuum, it is difficult to ascertain the state of aggregation in the original dispersion.

To ensure rapid and precise measurements of particle size as well as size distribution directly in dispersion, asymmetric flow field-flow fractionation was chosen to characterize nano-sized silver, gold and copper particles (upper Fig.). A method for the high-density particles was developed, including optimization of flow rates and carrier composition. The results are verified by image analysis obtained by EM analysis. In combination with UV/Vis absorption measurements, size distributions of the sols are correlated with optical absorption (lower Fig). Various preparation conditions are investigated and are especially dedicated to the presence of salts in the solvent. The particle stability was monitored over a more than two weeks.

(*C. Helmbrecht*)

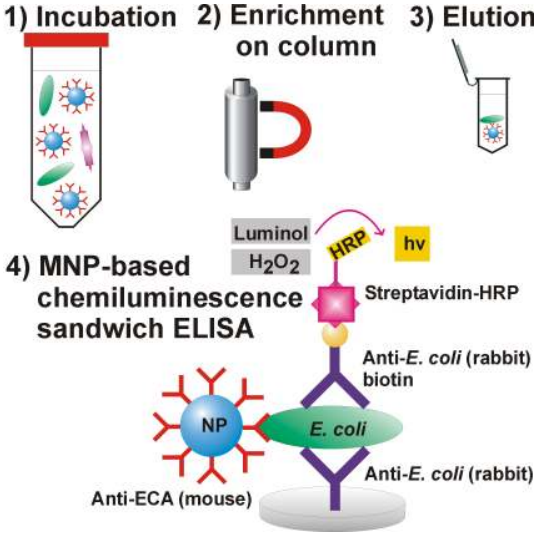
1.5 Bioseparation and Microarray Technology (Head: Dr. M. Seidel)

1.5.1 AQUASens: Immunomagnetic Separation and DNA Chip

Funding: BMBF
Cooperation: Siemens AG, München; FRIZ Biochem Gesellschaft für Bioanalytik mbH, München; Inge AG, IWW Rheinisch-Westfälisches Institut für Wasserforschung GmbH, Mülheim a.d. Ruhr; Technologiezentrum Wasser, Karlsruhe

A rapid online detection system for pathogenic microorganisms in water is developed within the AQUASens project. After a primary enrichment with microfiltration (dead-end microfiltration developed by IWW and cross-flow microfiltration developed by IWC), cells are selectively pre-concentrated with immunomagnetic separation (IMS) and quantified with a chemiluminescence-based DNA microarray.

Rapid methods for the quantification of pathogens are required for the monitoring of faecal contamination in water to secure public health. The IMS offers rapid enrichment and purification of bacteria in complex matrices. IMS has advantages over other pre-concentration methods, e.g. affinity columns, in terms of selectivity and flexibility of bacterial enrichment. By coupling different antibodies to the magnetic beads, the choice of target cells can easily be changed.



Immunomagnetic separation in combination with CL sandwich immunoassays for the quantification of bacteria

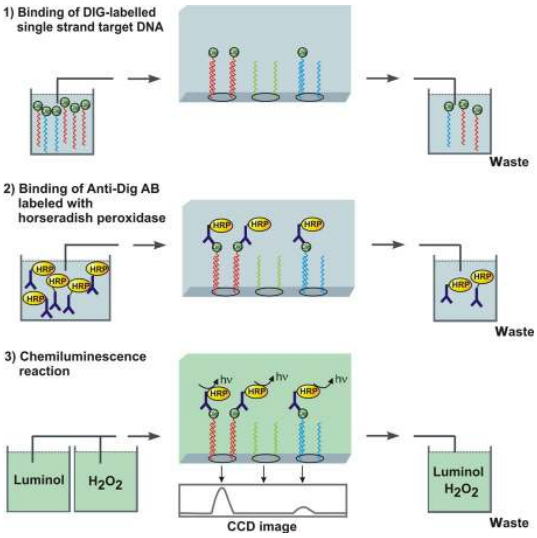
We developed a method for the production of magnetite particles (MNPs) for use with IMS, which is reproducible, cost-effective, and easy to perform. The particles had a diameter between 60 - 300 nm and were covalently coupled to antibodies that recognize an antigen common to all Enterobacteriaceae. Thus, a group-specific pre-enrichment of bacterial cells is possible, which can be combined with a species-specific analytical method. The synthesized particles were used along with commercially available magnetic columns for the selective immunomagnetic enrichment of E. coli from 10-mL water samples. The volumetric enrichment factor was 9. The enriched cells were analyzed with a MNP-based chemiluminescence sandwich ELISA. For enriched samples, the limit of detection was reduced from 5×10^6 CFU/mL to 2.6×10^5 CFU/mL. Using 200 μL anti-ECA-MNPs, we determined a recovery of 97±6% for a sample containing 10^6 CFU/mL and 89±2% for a sample containing 10^7 CFU/mL. The overall time for cell enrichment and detection was 3 h 45 min.

The nanoparticle-based method is an effective separation technique for water and food analysis. Its advantage over other methods is that it allows for the enrichment and purification of bacteria from complex matrices, especially from samples containing a large amount of particulate matter. The MNPs can be readily adopted for the enrichment of different bacteria by coupling them to other antibodies. A possible application is to combine this method online with a preceding primary enrichment and a following bioanalytical detection method such as PCR, immunoanalytical and DNA microarrays or our automated platform for chemiluminescence flow-through microarrays.

We have developed a hybrization assay on DNA microarrays for the quantification of amplification products of the hipO gene of Campylobacter jejuni, the hilA gene of Salmonella typhimurium and the stx1A gene of E. coli O157:H7. Using the stopped-

PCR strategy, the amplified target DNA was strongly dependent on the applied gene copies. The quantification is carried out by a flow-through chemiluminescence microarray readout system. The DNA microarrays are based on a poly(ethylene glycol)-modified glass substrate. The probes on the surface are 20 nucleotides long and the quantified PCR product 60 nucleotides. The amplification is stopped after 35 cycles, at this point amplification was in the middle of the logarithmic phase and the spread between different DNA starting concentrations reaches a maximum.

The chemiluminescence DNA microarray is very fast and sensitive if used with single stranded DNA as the analyte. The assay time is 15 minutes and the limit of detection is 40 copies/mL. These facts implicate that the two strands synthesized by PCR amplification should be separated prior to the hybridization assay on the DNA microarray. As the reverse primer is already labeled with biotin a separation using streptavidin labeled microbeads preceding the hybridization assay is a fast way to separate the strands. In addition the forward primer is labeled with digoxigenin for binding a HRP-antibody conjugate to generate the chemiluminescence signal. These variations reduce the assay time for the hybridization assay with double stranded PCR product from 7 hours to 2 hours and dramatically increase the sensitivity.



CL immunodetection of single strand generated PCR products

The detection limit for the gene hipO of C. jejuni was 2 cells/mL, for the gene hilA of S. typhimurium and the gene stx1A of E. coli O157:H7 it was 14 cells/mL. This system allows for a sensitive detection and quantification of all three bacteria in a concentration range from 100 to 1000 cells/mL.

The developed method combines the strong and fast amplification of nucleic acids by PCR and the sensitive detection of nucleic acids by a DNA microarray in a way that allows not only the sensitive detection of bacterial DNA but also its quantification. The method is adjustable to meet the requirements of the legal limits.

However, the legal regulations in Germany requires the detection of a single cell per 100 mL of drinking water. In order to meet this demand and to achieve levels of bacteria detectable by the presented technique, sample preconcentration steps will be necessary prior to analysis. Consequently, for the flow-through chemiluminescence microarray readout system to be used in water monitoring, the system will have to be integrated in an inline setup with preenrichment modules, such as microfiltration and immunomagnetic separation. In this way detection times would increase, but the common microbiological enrichment methods still take much longer and are more laborious. Furthermore for this application, an extension of the detectable gene spectrum would be important. The active area of the chip still offers considerable free space for this. Hence, an integration of a variety of additional DNA probes is possible on the presented platform. Multiplexed experiments in drinking water are the next step towards exploiting the power of the chemiluminescence DNA microarray for pathogenic bacteria detection in water.

(*G. Pappert, S. Donhauser*)

1.5.2 Development and Testing of a Multianalyte Platform for High-throughput Analysis in Food Control Based on a Chemiluminescence Flow-through Microarray Chip

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

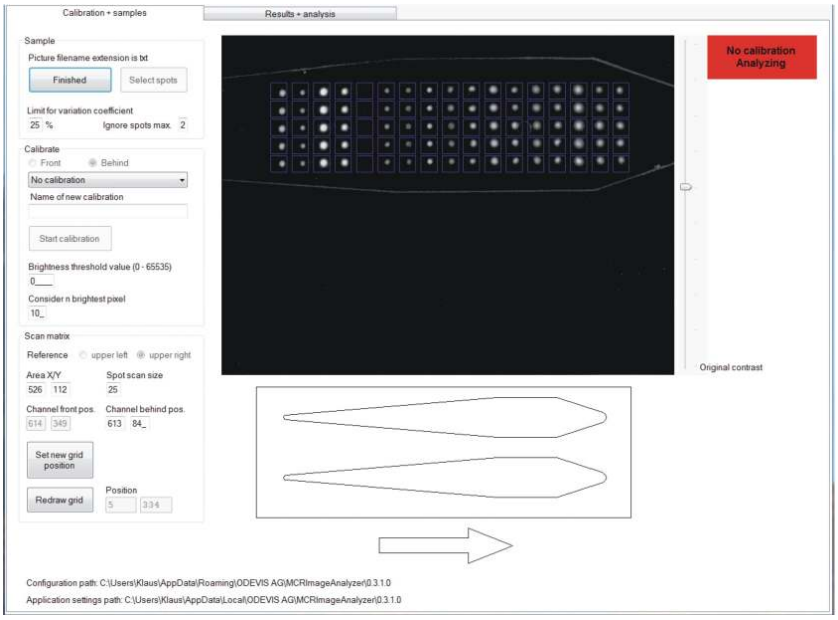
The stand-alone platform MCR 3 (Munich Chip Reader, 3rd generation) is able to quantify multiple analytes in complex matrices of food and liquid samples for field analysis or for routine analytical laboratories. The MCR 3 is a self-contained system for fully automated multiplexed immunoanalysis: the flow-through microarray chip, the temperature-controlled microfluidics and the software module enable automated calibration and simultaneous determination of different analyte concentrations during a whole working day.

At the IWC we are currently engaged in the cost-effective manufacturing of flow-through microarray chips and the optimization of the fluidic system of the new generation of the MCR 3, like the cooling and handling of the antibody syringe unit, the durability of the turning valves, the driven control of the syringe pumps and the operation and treatment of the piping systems and the storage reservoirs.

Another task is the development of an user-friendly fully automated data analysis of microarray images for a routine application. Therefore we develop an application software which identifies the single light spots including standard deviation and outliers for generating reproducible standard calibration curves to analyze several food matrices.

Utilizing the obtained calibration data, the software is able to perform fast determination of residues in food samples with respect to type and concentration of the contaminants. Exceedings of the valid maximum residue limits (MRLs) are highlighted in order to allow a fast rating of samples in the measurement routine.

The figure illustrates the graphical user interface of the MCR 3 for the multiplexed analysis of chemiluminescence microarray images.
(*K. Kloth, K. Wutz*)



Graphical user interface of the MCR 3

1.5.3 Validation of the Munich Chip Reader (MCR 3) for the Analysis of Antibiotics in Raw Milk Samples

Funding: BayStMELF (Bavarian State Ministry for Nutrition, Agriculture and Forestry)
Cooperation: Chair of Hygiene and Technology of Milk, Prof. Märtlbauer, LMU München; Milchprüfring Bayern e.V., Wolnzach; MUVA, Kempten

The availability of high-quality and savfe food is a basic demand in our society. The European Union has defined maximum residue levels for a number of antibacterial compounds. As methods for rapid and inexpensive qualification and quantification of these compounds are lacking, a chemiluminescence read-out system MCR 3 for analytical flow-through microarrays based on multiplexed immunoassays has been developed.

The regenerable antibiotic microarray chips based on PEG-ylated surfaces are currently used for the parallel analysis of 14 different antibiotics in milk within 6 minutes. Microspotted antibiotic derivatives like sulfonamides, β-lactams, aminoglycosides, fluorquinolones and polyketides are directly coupled to epoxy-activated PEG chips without further use of linking agents. Using the MCR 3 platform, this antigen solid phase was stable for at least 50 consecutive analyses. Calibration experiments ($m = 5$, $n = 8$) were successfully carried out as illustrated in the map. Overall, the new microarray system offers the potential of inexpensive identification and quantification of antibiotics and will aid the food industry to maintain quality and safety of milk.

The practical applicability is tested in a service routine laboratory at the Milchprüfring Bayern e.V. yielding an excellent precision of the method. The β-lactam penicillin G is the most detected antibiotic in real raw milk samples (73%) in the range of 5 - 30 μg/L ($m = 100$) followed by cloxacillin (17%) and ampicillin (6%).

	TMP [µg/L]	WR [µg/L]	MRL [µg/L]
SMA	15,3	2,8 - 233	100
SDA	17,2	2,3 - 426	100
Streptomycin	15,2	3,3 - 171	200
Cloxacillin	0,8	0,03 - 112	30
Ampicillin	6,6	1,5 - 67	4
Penicillin G	19,3	3,8 - 253	4
Cephapirin	1,6	0,4 - 18	60
Neomycin B	1,8	0,2 - 76	1.500
Gentamicin	10,8	4,1 - 51	100
Erythromycin A	1,2	0,1 - 116	40
Tylosin	5,2	1,9 - 25	50
Enrofloxacin	0,5	0,1 - 6	100
Nafcillin	1,5	0,2 - 55	30
Ceftiofur	2,9	0,5 - 51	100

Table of 14 calibration experiments on one microarray chip (TMP = test midpoint, WR = working range, MRL = maximum residue level)

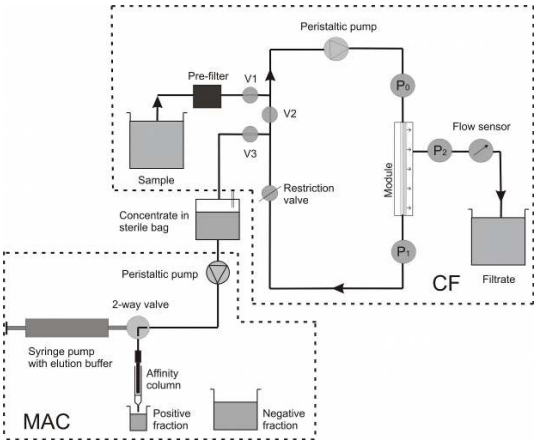
The Chair of Hygiene and Technology of Milk is working on the development and production of the specific primary antibodies used for the CL-MIA. The MUVA Kempten is responsible for the reference analysis method based on liquid chromatography and mass spectrometry.

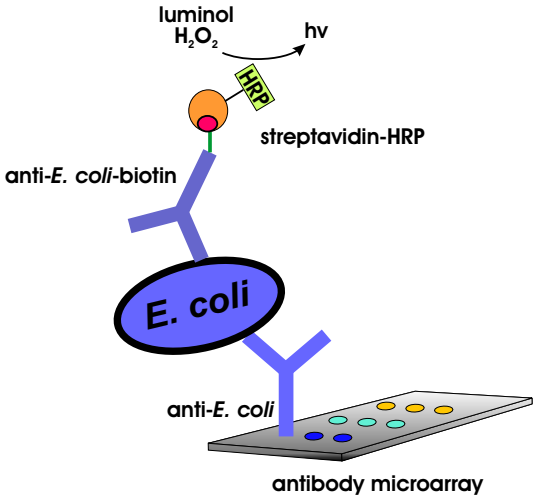
At the IWC we are currently engaged in the fabrication and the validation of the multi-use antibiotic microarray chips. The operational microarray flow cells are stable for about 2 - 3 months by storing them at -18°C in order to assure a sufficient light intensity for all detectable antibiotics. The average interassay variance of the produced microarray chips ($m = 5$, $n = 12$) is about 4%. (*K. Kloth*)

1.5.4 Combined System for Enrichment and Detection of Microorganisms in Drinking Water

Funding: DFG

Pathogen detection is important for health and safety reasons. Several outbreaks all over the world have shown the need for rapid, quantitative, and particularly multianalyte detection systems. Escherichia coli serves as hygiene indicator and have to be included on a microarray which quantifies waterborne pathogens. A rapid method which quantifies Escherichia coli down 1 cell in 100 mL in 1 - 4 h is required for the monitoring of faecal contamination in water and is the aim of this project. The combination of a primary enrichment, followed by a selective enrichment and purification of bacteria and a subsequent multi-analyte detection of different bacteria could be used for monitoring of microorganisms in water. This combined system is the aim of the present work, whereas the experiments have been carried out with living E. coli (DSM 1116) until now. Enrichment is performed by cross-flow filtration and followed by the selective enrichment using a monolithic column or immunomagnetic separation. For the detection antibody microarrays are used.





For the enrichment of microorganisms a closed two-step process is developed. It consists of a cross-flow filtration (CF) and a monolithic affinity column (MAC) combined with a sterile bag. The computer-controlled CF system is made up of a peristaltic pump, magnetic valves and a hollow fiber membrane module. The peristaltic pump creates a transmembrane pressure (TMP) through the hollow fiber module and can be adjusted by the restriction valve. The TMP can be controlled online with pressure sensors. With the magnetic valves the three steps filling, concentration and elution can be set. The concentrate (50 mL) is eluted directly to the sterile bag and acidified to pH 4. With a second peristaltic pump, the pre-enriched microorganisms are pumped through the monolithic affinity column. On the monolithic affinity column the affinity ligand Polymyxin B (PmB) is immobilized. The interaction between PmB and gram negative bacteria is electrostatic. With the pH-value of 4 the bacteria are retarded. The elution is carried out by increasing the pH-value to 8.2.

The principle of the detection with antibody microarrays is based on a sandwich ELISA, which is transferred to the microarray platform. The microorganism-specific immobilized antibodies serve as capture molecules. The antibody microarrays are produced on polyethylene glycol modified glass surfaces. For the recognition step, specific biotinylated detection antibodies are used, which are bound by a steptavidin-horseradish peroxidase conjugate. The enzyme generates photons by a chemiluminescence reaction which is recorded by a CCD camera.

The main focus layed on the detection of living E. coli. For the measurement of living bacteria different conditions were tested and optimized. With regard to the importance of combining the enrichment and detection step, first experiments were carried out to detect E. coli after the enrichment by immunomagnetic separation (IMS). Here it was

shown, that the detection was possible after IMS. Currently the parallel detection of different water relevant bacteria on the microarray is prepared. Here it is important to test different antibodies to determine the best antibodies for further use. Also the combination of the microarray detection with cross-flow filtration and the monolithic column is planned and will also be used for the analysis of different environmental water samples.
(*V. Langer, S. Ott, G. Pappert*)

1.5.5 Detection of Staphylococcus aureus and Bacillus cereus in Milk Products After Enrichment with Bioaffinity Columns

Funding: Arbeitsgemeinschaft industrieller Forschungsvereinigungen (AiF); Forschungskreis der Ernährungsindustrie (FEI)
Cooperation: Chair of Hygiene and Technology of Milk, LMU München; Institute for Food Chemistry, University Hamburg; Chair for Fluid Mechanics, Friedrich-Alexander-University Erlangen-Nürnberg

For companies in food industry the quality of products is essential to be competitive and powerful in the economy. To save the consumers health it is important to detect losses in quality as soon as possible. For milk and dairy products two indicator microorganism are important. Staphylococcus aureus indicates the efficiency in process hygiene and Bacillus cereus plays an important role for the identification of putrid dairy products. With the official methods negative results are received after 24 h for Staphylococcus aureus and 48 h for Bacillus cereus, respectively, and the confirmation of positive samples lasts up to 144 h. For biomolecular methods it takes at least 12 - 24 h for the detection in food samples.

Image of a monolithic affinity colum

Therefore, a faster method for the detection of Staphylococcus aureus and Bacillus cereus, using a full automated microarray chip reader, is developed. A detection limit of 100 cells/spores per mL should be reached by means of antibody microarrays. To get these concentrations, the microorganisms have to be enriched from milk. This is possible with a monolithic affinity column. Because of its coherent network of pores, where microorganisms can pass easily, high flow rates can be reached resulting in low back pressures. The used monolith is produced by self-polymerization of the monomer polyglycerol-3-glycidylether with the Lewis acid BF_3 and the porogens toluene and tert-butyl-methylether. After polymerization, the epoxy groups are activated and coupled to aptamers or antibodies against Staphylococcus aureus and Bacillus cereus. With those receptors, the microorganisms can be captured and separated from the matrix molecules in milk. After elution of the analyte molecules the column should be regenerated and used again. The parameters of the column like geometry, porosity and pore size have to be optimized by CFD modeling. The optimal geometry of the column obtained by experiments has an inner diameter of 11.8 mm and a reaction volume of 400 μL. With that, back pressures of 0.81±0.06 bar are achieved for flow rates of 20 mL/min. For those flow rates, it is possible to enrich Staphylococcus aureus and Bacillus cereus in 1 L milk within 1 hour.
(*S. Ott, V. Langer*)

1.5.6 Pathogenic Viruses in Water – Detection, Transport and Elimination

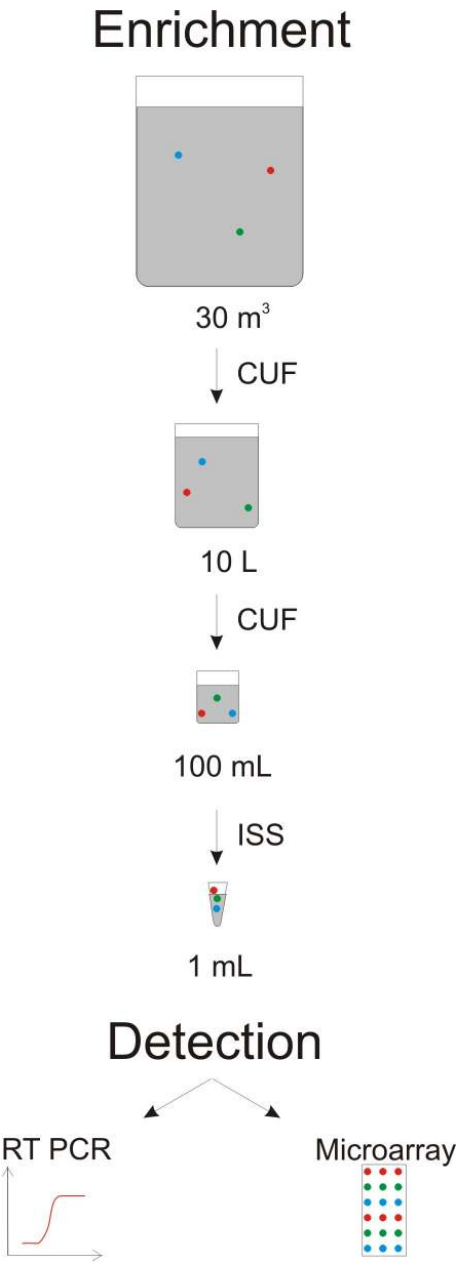
Funding: DFG
Cooperation: Centre of Infectiology and Infection Prevention, University of Bonn; Federal Environment Agency, Berlin; Institute of Groundwater Ecology, Helmholtz Zentrum München; Institut für Siedlungswasserwirtschaft und Abfalltechnik, Leibniz University of Hannover

Viruses are one of the most dangerous contaminants in water. Mainly enteroviruses (Polioviruses, Coxsackie virus A and B, ECHO virus), Norwalk or Norwalk-like viruses, Rotaviruses, Hepatitis E and A virus and Adenovirus belong to the health-relevant water-associated viruses. In order to avoid the outbreak of water-borne diseases caused by such viruses, it is necessary to have a system for monitoring samples quickly and sensitively.

Detecting water-borne viruses is much more complex than the detection of other microorganisms. Many viruses are only poorly culturable and when these cultivation methods are possible, it takes a lot of time until getting results. Furthermore, viruses are able to cause diseases in very low concentrations. So, in this project a system, which combines the enrichment of viruses out of 30 m^3 water with the detection and quantification, will be developed For first experiments, the bacteriophage MS2 will be used, representative for RNA phages. Afterwards phiX174 will serve as a model system for somatic phages.

The system should consist of a cross-flow ultrafiltration (CUF), monolithic affinity chromatography and a DNA-microarray system, combined with a multiplex PCR assay. The cross-flow filtration should be able to enrich viruses from large volumes (30 m^3) to a volume of about 10 L in the first and 50 - 100 mL in a second step. With monolithic columns based on porous polymers a further immunoselective separation should be possible. The resulting small volumes of about 1 mL can then be utilized for detection. For identification and quantification a flow-through chemiluminescence DNA microarray system will be developed. This chip should be combinable with the DNA microarray developed for the quantification of microorganisms in water. Furthermore a reverse transcription real-time PCR assay has to be designed. It will be used for amplifying the viral RNA for microarray detection and moreover for the determination of recovery rates in filtration experiments.

With the combination of these methods monitoring of drinking-water should be able within hours.
(*S. Prell, M. Rieger, S. Ott*)

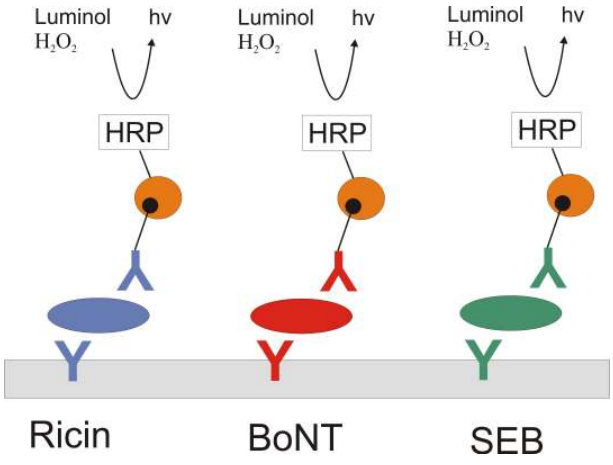


Schematic design of the two-stage CUF process combined with affinity capturing of viruses followed by quantitative analysis of DNA by real-time PCR or analytical microarrays

1.5.7 Development an Antibody Microarray for the Detection of Toxins

Funding: IWC
Cooperation: Robert-Koch-Institut, Berlin

High molecular-weight proteotoxins such as ricin, botulinum neurotoxins (BoNT) and staphylococcal enterotoxin B (SEB) are regarded as potential biological warfare agents. These toxins could be used for bioterroristic attacks, because of their availability, ease of preparation, stability and high toxicity. Contamination of water, liquids or food with toxins demonstrates a precise danger for the civil population. The currently used methods for the detection of toxins are time consuming. Currently, fast detection systems lack sensitivity. Therefore high sensitive, specific and fast multi-analyte test systems are required.



Schematic of the microarray for toxins

Within the scope of the cooperation with the RKI Berlin the antibodies, which showed the best sensitivities on the Luminex system are to be tested with the Munich Chip Reader 3. Our results will be compared to these of the RKI, reached with their device. Here, importance will be attached to limit of detection, assay length and reagents consumption.

At the IWC an assay system using antibody microarrays is to be developed for detecting toxins. The quantification of the proteotoxins will be implemented using a sandwich immunoassay. Monoclonal and polyclonal antibodies are immobilized covalently on polyethylene glycol substrates, which capture toxins out of liquid samples like water, milk, juice etc. Specific detection antibodies labeled with biotin bind to the antigen, followed by addition of streptavidin marked with horseradish peroxidase. The detection is carried out by a catalyzed chemiluminescence reaction, which is recorded by a CCD camera.

The measurements are carried out on the MCR3 platform, whereas the optimization of measuring conditions such as flow rates, exposure time respectively insertion of time range spacing and amount of antigen and antibody, in order to minimize the antibody consumption play an important role. In this context the optimization of storage terms for long-time application of the produced antibody microarrays will also be done.
(*A. Skola*)

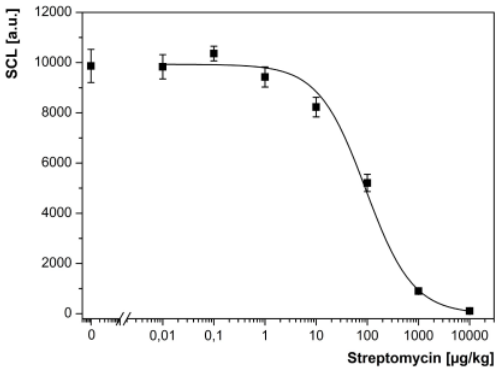
1.5.8 Quantification of Antibiotics in Honey with the Munich Chip Reader 3

Funding: IWC

Honey is generally considered as a natural and healthy product. However, treatment of bacterial brood diseases in apiculture (e.g. American foulbrood disease) and the abatement of the plant disease Fireblight can cause contamination of honey with antibiotic residues. The presence of antimicrobial residues in food hold the risk of undesirable human health effects, e.g. allergic reactions, and the occurrence of bacterial resistance to antibiotics. Regarding the European legislation (EU Regulation 2377/90), no antimicrobial residues in honey are allowed (zero tolerance).

The quantification of antibiotics in honey is based on an indirect competitive ELISA on a microarray platform. The antibiotic derivatives are immobilized on a PEG-ylated biomimetic glass surface. For an automated flow-through chemiluminescence read-out the MCR 3, which has been developed at the IWC for the rapid and simultaneous online detection of 14 different antibiotics in milk, is used. For CL-MIA measurements a regenerable microarray chip is used, which allows up to 50 consecutive measurements with one chip.

Due to the high viscosity of the matrix, the honey samples have to be diluted 1:10 (w/w) in PBS solution before injection in the fluidic system of the MCR 3. To avoid recrystallisation of sugar in the tubes and valves the rinsing program of the MCR 3 after the CL-MIA measurement has been optimized for the honey matrix by monitoring residues of glucose in the tubes. The resulting measurement and rinsing program for the quantification of antibiotics in honey samples takes 13:45 minutes. This guarantees the requested fast multi-analyte screening.



Calibration curve for Streptomycin

Up to now, we can quantify the antibiotics sulfamethazine between 52 and 1712 μg/kg, sulfadiazine (33 - 4382 μg/kg), streptomycin (34 - 712 μg/kg) and enrofloxacin (4 - 20 μg/kg) in parallel. The resulting working ranges allow efficient monitoring of maximum residue levels, which are valid for other food of animal origin as documented in EU regulation 2377/90.

Due to the loss of CL signal intensity with increasing number of measurements with one chip, a correction factor was developed for the determination of the recovery. With means of this signal correction, sufficient recovery rates for spiked samples within the particular working ranges can be obtained in dimensions between 91% and 135%.

(*K. Wutz*)

1.6 Aerosol Research (Head: Prof. Dr. R. Niessner)

1.6.1 Emissions of PAHs, Nitro-PAHs and Carbonyl-compounds During the Combustion of Biofuels and Biofuel Mixtures

Funding: Fachagentur Nachwachsende Rohstoffe (Federal Agency for Renewable Resources)
Cooperation: Prof. Schramm, Institute of Ecological Chemistry, Helmholtz Zentrum München; Prof. Hausberger, Institute of Combustion Engines, TU Graz; Prof. Geringer, Institute of Combustion Engines, TU Vienna

There is a limit of supplied fossil oil, originated from underground, which can be applied as fuel. Also an enhancement in the greenhouse effect, hence earth atmosphere heating, implies that alternative energy sources are needed. By use of biofuels and biofuels blends, it is possible to partially substitute fossil fuels. Though, up to now, besides the still open questions on the use of arable land to produce biofuels, there is just little knowledge about in which extent the addition of biofuels to fossil fuels will change the emission rates of PAHs, nitro-PAHs and carbonyl compounds during engine combustion.

Sampling setup at the rolling test stand in Vienna

To get more detailed information on the emission rates of the different engine exhaust components, samples were taken after dilution tunnels at vehicle roller test benches in Graz and Vienna during defined test cycles. An heavy duty vehicle (MAN, EURO V), a tractor motor (John Deere, EU III) as well as passenger cars (Audi, diesel, EURO V and Saab, gasoline, EURO IV) have been used during this study. To determine differences in the emission rates, fossil diesel, biodiesel and vegetable oil as well as mixtures with different amounts of biofuels in fossil fuel were investigated. Particle-bound PAHs and nitro-PAHs were sampled on quartz fiber filters, which were extracted and cleaned up for laboratory quantification by HPLC-FLD. The gaseous carbonyl compounds were collected with gas washing bottles using a solution of dinitrophenylhydrazine in acetonitrile and were detected by HPLC-UV.

As regards the concentration of PAHs and carbonyl compounds between the different types of fuel investigated in this study, fossil diesel and fuel blends with low level of biodiesel (up to 10%) show very similar values among each other. Differences are recognized when pure vegetable oil is directly compared to fossil diesel fuel. In this case, higher values are found of PAHs and carbonyl compounds concentrations compared to those obtained when operating with fossil diesel fuel alone. As regards the gasoline engine tested, the addition of ethanol does not produce significant variations in comparison to the operation with pure gasoline

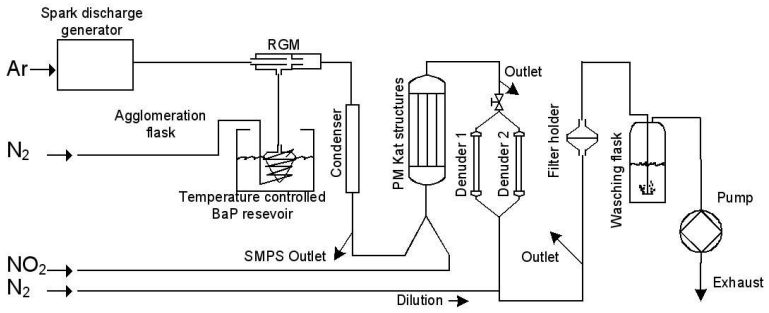
Concerning nitro-PAHs, different vehicles have an individual response to the fuels used for the tests. As regards diesel engines, results show again that fuel blends with low content of biodiesel have no different emission in any of the vehicles in comparison to fossil diesel. On the other hand emissions from pure biodiesel, pure vegetable oil or a mixture of them and fossil diesel fuel, present significant reductions in comparison to fossil diesel fuel in the tractor engine. Nevertheless they remain unchanged in the MAN truck and in the Audi passenger car. Regarding the gasoline engine, the addition of ethanol has a positive effect. Indeed the nitro-PAH emissions are noticeably reduced by adding moderate quantities of ethanol (up to 10%).
(*M. Knauer, M. Carrara*)

1.6.2 Nitro-PAH Formation in Diesel Particulate Filters

Funding: DFG

Diesel particulate matter is widely considered as a possible human carcinogen. It represents a complex mixture of organic and inorganic materials where the inorganic part mainly consists of fine soot particles produced during the high temperature combustion of fuel. Several classes of organic components such as polycyclic aromatic hydrocarbons (PAHs), nitrated PAHs (nitro-PAHs) and aliphatic hydrocarbons can adsorb on the soot surface. PAHs are often already present in the fuel and they may survive the combustion process while others undergo de-novo formation. On the other hand, nitro-PAHs are formed during the combustion via electrophilic substitution in presence of NO_2. Nitro-PAHs have been found to account for over 50% of the total vapor and particle phase direct mutagenicity of ambient air and particulate matter; the carcinogenic character of diesel soot is mainly attributed to nitro-PAHs.

Diesel particulate filters (DPF) have evolved to a promising technology to reduce harmful diesel emissions. They are typically ceramic monoliths produced with alternating flow channels, which are closed at the ends to force the exhaust flow to pass through the porous wall of the honeycomb filtration media. The solid particles deposit in the pores. These filters became plugged soon by the soot that they trap and this leads to an increase of the back-pressure that compromises the correct engine running. Therefore, it is necessary to regenerate the filters periodically at elevated exhaust temperature. Often, the exhaust gas is first passed through a diesel oxidation catalyst designed to convert NO to NO_2 which is used to assist the filter regeneration by enhanced soot oxidation. Considerable amount of PAHs may reside on the soot particles and the filter structure could support the nitration chemistry leading to a post-combustion formation of nitro-PAHs. Heterogeneous gas-particle degradation of PAHs has already been studied and real DPFs have already been tested with respect to nitro-PAH formation. Nevertheless, information on the nitration kinetic with a focus on reaction products and under conditions relevant for diesel aftertreatment systems are still missing.



Simulated diesel exhaust aftertreatment system

Our experiments deal with the interaction of artificially pyrene- or benzo(a)pyrene-coated spark discharge particles with NO_2. A sub-monolayer PAH coating was selected to simulate the adsorption conditions of semi-volatile PAHs in a diesel exhaust tailpipe system. The heterogeneous reactions of adsorbed PAH with NO_2 have been investigated over a wide range of conditions relevant for diesel exhaust specifications. For pyrene (PYR) coated soot 1-nitropyrene (1-NPYR) has been found as the main nitration product. Its production is linearly correlated with the reaction time. The 1-NPYR formation rate increases exponentially with NO_2 concentration which is indicative of the underlying reaction mechanism being not a simple one. Looking for the effects of temperature, we found the highest 1-NPYR concentration on particles at 100°C while at temperature above 200°C, the 1-NPYR amount found was comparable to that found at 20°C. Probably at high temperature the educt (PYR) and/or the product (1-NPYR) desorb into the gas-phase. Benzo[a]pyrene (BaP) is even more re-

active than PYR towards nitration. In experiments on quartz filters, ca. 75% of coated BaP is converted to 6-nitrobenzo(a)pyrene (6-NBAP) after 3 hours. In our simulated diesel exhaust after treatment system (in the figure) we found the formation of 1- and 6-NBAP. Formation rate was higher at 150°C and decreased at higher temperature.

We demonstrate that under conditions relevant for DPFs production of 1-NPYR, 6-NBAP and other nitro-PAHs is possible. Running experiments at the MAN test stand in Nürnberg with a commercial heavy duty engine coupled with a DPF will add more information on the topic.
(*M. Carrara, J. Wolf*)

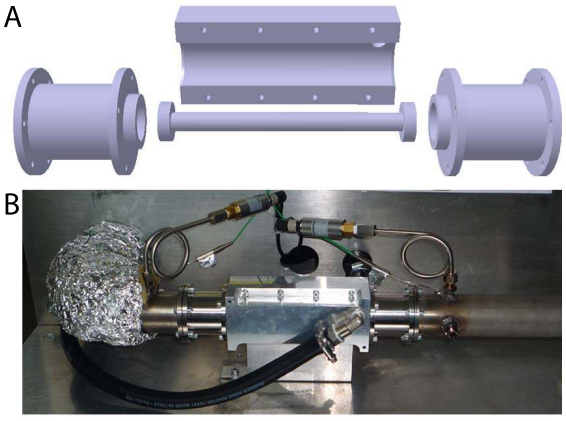
1.6.3 Analysis of deposition mechanisms on the gas side surface of exhaust gas heat exchangers

Funding: Forschungsvereinigung Verbrennungskraftmaschinen (Research Association for Combustion Engines)
Cooperation: Prof. Wachtmeister, Institute for Internal Combustion Engines, TU München

Nitrogen oxide (NO_x) emissions from diesel powered vehicles are regarded as hazardous air pollutants. For this reason NO_x emissions are legally limited and the maximum permissible value will be set to an even lower level in the near future.

One method for the reduction of NO_x realized by the automotive industry is cooled exhaust gas recirculation (EGR): the temperature of a fraction of the exhaust gas is reduced in a water-cooled heat exchanger, then it is mixed with fresh charge air and returned to the engine. Thus, the combustion temperature is lowered and less NO_x is produced. However, soot particles emitted from the engine are deposited inside the exhaust coolers on the gas side surfaces, thus causing the heat transfer efficiency to drop as well as the pressure losses to increase.

To establish a better understanding for the deposition mechanisms involved in EGR heat exchangers, the existing model test bench was further improved. It is now possible to create a soot aerosol that not only in its size distribution but also in its composition is comparable to real diesel exhaust gas. This is achieved by adding water, diesel components and sulfuric acid and the soot formed in a propane gas burner to a hot gas flow ($T_{gas} > 400$ °C).



A newly constructed test heat exchanger was integrated in the bench which consists of only one single, exchangeable tube within the cooling jacket (see figure). This setup allows in the conduction of extensive experimental series to use always a clean tube.

To study the influence of varying conditions on the deposit build-up, different aerosol compositions were tested. It was found that condensation of non-volatile components significantly contributes to the deposition inside the tubes. In contrast, the condensation of water vapor helps to keep the gas side surfaces clean.

For the determination of the layer thickness of the deposited soot neutron radiography was used. This method has the advantage of gaining the required information in a non-destructive way. The neutron absorption measurements were conducted with the fouled heat exchanger tubes at the Heinz Maier-Leibnitz neutron source, Garching, using the ANTARES facility.

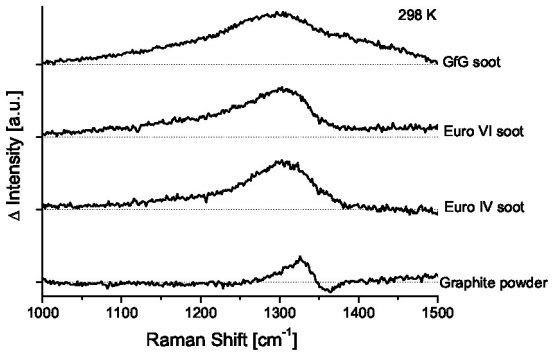
The results obtained from this measurements support the observations made during the test bench experiments.

The deposits generated in experiments at the engine test bench of the Institute for Internal Combustion Engines were analyzed for carbon, calcium and sulfate content. An increased organic carbon content (55%) compared to soot sampled on quartz fibre filters (10%) was determined in the samples. The presence of sulfates as well as fuel and oil additive components like calcium in the deposited soot underlines the importance of condensation in the deposit formation. However, explicit modeling of the mechanisms is still on the way.
(*G. Hörnig*)

1.6.4 Analysis of Soot Structure and Reactivity Based on the Dispersive Character of D Mode in Raman Spectra

Funding: DFG
Cooperation: Prof. Schlögl, Fritz-Haber-Institute of the Max-Planck-Society, Berlin

Soot is defined as the black solid product of incomplete combustion or pyrolysis of fossil fuels and other organic materials. In urban areas, diesel soot particles account for the major fraction of fine air particulate matter. The importance of information about soot structure and reactivity significantly increased in recent years, since the development of modern diesel engines can result in more reactive soot particles. The knowledge about structure and reactivity of soot can be used for the investigation and optimization of diesel exhaust aftertreatment systems. Moreover, this information can help us to understand the influence of soot particles on the environmental chemistry, climate, and public health. High Resolution Transmission Electron Microscopy (HRTEM) is usually applied for the investigation of soot structure, whereas the reactivity of soot is normally determined by Temperature Programmed Oxidation (TPO). However, HRTEM and TPO measurements are too demanding for routine analysis. Therefore it is highly desirable to establish an analytical tool that allows for rapid determination of the soot structure and reactivity.



Difference Raman spectra for different soot types

Raman Microspectroscopy (RM) provides fingerprint spectra and allows us to obtain detailed information about reactivity of different soot samples by determining their structure. The soot spectra show peaks at ca. 1580 cm^{-1} (G or Graphite peak) and 1350 cm^{-1} (D or Defect peak), but the D and G peaks exhibit strongly varying relative intensities and widths that can be used for structural characterization. Moreover, for different graphite and soot samples the D mode is dispersive, while the position of the G peak is invariant. The dispersive character of the D mode (i.e., the shift with the excitation energy, at the rate of 40–50 cm^{-1}/eV over a wide range of λ_0) is the well-known effect found in different kinds of carbon materials. This effect has been attributed to double-resonant Raman process.

In order to compare the behavior of D mode for untreated and oxidized Graphite powder, EURO IV, VI and spark discharge generated (GfG) soot, we calculate the differences of spectra measured at 514 nm and 633 nm (see figure). As expected, the smallest differences are found for untreated graphite powder. The difference spectra of EURO IV and VI are characterized by similar intensities and widths (about 1000 - 1400

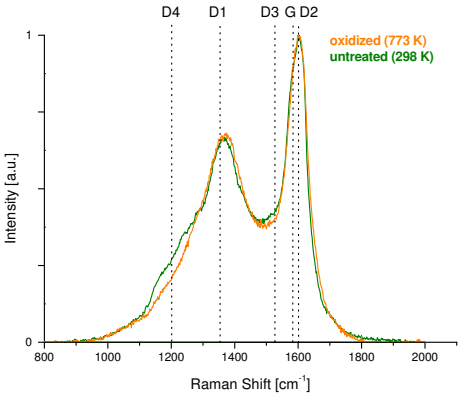
cm^{-1}). The untreated GfG soot shows largest differences in spectra (from ca. 1000 to 1500 cm^{-1}) obtained with Ar and He-Ne lasers. Obviously, the growing differences in spectra of graphite, EURO IV and VI, and GfG soot measured at 514 and 633 nm can be explained by increasing degree of disorder and/or molecular content from graphite powder to GfG soot. In the oxidation experiments, no significant changes are found in the difference spectra of graphite powder and EURO IV and VI soot samples before and after oxidation. Oxidized GfG soot reveals lower intensity in the difference spectrum (as compared to untreated GfG soot and EURO IV and VI soot samples), which indicates significant increase in the structural order of GfG soot during oxidation. We plan to perform more detailed structural analysis of soot based on the dispersive character of the D mode. This will be implemented using the new Raman Microscope equipped with 3 excitation lasers (532, 633 and 785 nm).
(*M. Knauer, N. P. Ivleva, J. Schmid*)

1.6.5 Characterization of Soot Reactivity by Temperature Programmed Oxidation and Raman Microspectroscopy

Funding: Forschungsvereinigung Verbrennungskraftmaschinen
Cooperation: Prof. Pischinger, Institute of Combustion Engines, RWTH Aachen

Substantial reduction of anthropogenic aerosol exhaust is mandatory for the overall air quality. Highly populated areas with heavy traffic are especially affected by the emission of combustion aerosols. Soot particles emitted by diesel engines provide the major fraction of air pollutants and hence must be prevented from leaving the exhaust system. Therefore, a wide range of particle trapping systems and exhaust aftertreatment technologies are currently under investigation. The necessary regeneration step of such particle traps can be promoted by highly reactive soot.

Experiments concerning the reactivity of soot are done by Temperature Programmed Oxidation (TPO). High Resolution Transmission Electron Microscopy (HRTEM) is usually applied for investigation of soot structure. However, TPO and HRTEM measurements are very time and cost consuming. On the other hand, one can obtain detailed information about the reactivity of soot by measuring the structure with Raman Microspectroscopy (RM).



Raman spectra of untreated and oxidized soot

RM provides fingerprint spectra with spatial resolution of optical microscope. RM has been applied for the structural characterization of different diesel soot samples. Raman spectra show peaks at ca. 1580 cm^{-1} (G or Graphite peak) and 1350 cm^{-1} (D or Defect peak), but the D and G peaks exhibit strongly varying relative intensities and widths. For the quantitative spectral analysis we applied a five-band fitting procedure with combination of four Lorentzian-shaped bands (G, D1, D2, D4 at ca. 1580, 1350, 1620 and 1200 cm^{-1}) and one Gaussian-shaped band (D3 at ca. 1500 cm^{-1}). As the reference for reactivity limits, we used spark discharge generated soot (GfG) as upper limit (65% mass conversion) and a commercially available graphite powder (Graphite) for determination of lower limit (1-2% mass conversion). With this data the reactivity index (RI) was calculated, setting the GfG at RI:100 and Graphite at RI:0.

The RI allowed us to compare our TPO findings with our project partner's Thermogravimetric Analysis (TGA). Although the collection and the analytical method were different, the RI allowed a good correlation between both data sets. Within this project many different types of soot obtained for different combustion regimes were investigated (variable parameters were rotations per minute, fuel-to-air ratio and injection time). Furthermore, each operation point was analyzed with or without a Diesel Oxidation Catalyst (DOC). The provided reference und experimental engine operating points always showed decreased reactivity when the DOC was installed. This was in perfect agreement with the information derived from the Raman spectra. The influence of the fuel-to-air ratio on the reactivity was less dominant than the presence of the catalyst. Some samples collected during fuel-rich combustion and without a DOC showed strong signals in the D4 area which decreased upon oxidation (see figure). However, the lean combustion created more reactive soot for all the investigated engine operating points. These soot samples were characterized by higher amount of disordered graphitic structures and amorphous carbon (higher values for FWHM D1 and relative intensity of D3, respectively). The change of these parameters upon oxidation validates the findings of the absolute values.

Thus, RM provides information about structural order of graphitic and amorphous carbon fractions and can be used to analyze soot oxidation readiness.
(*J. Schmid, M. Knauer, N.P. Ivleva*)

2 Publications of Present Members of the IWC

2.1 Journal articles (reviewed)

S. Donhauser, R. Niessner and M. Seidel; Developing a Stopped-PCR Strategy for the Quantification of E. coli on a Flow-through Chemiluminescence Microarray Readout System. Anal. Sci. 25 (2009) 669-674

B. Fall and R. Niessner (2009); Detection of Known Allergen-specific IgE Antibodies by Immunological Methods. In: Microchip Methods in Diagnostics, ed. by U. Bilitewski. Vol. 509, Methods in Molecular Biology. Humana Press, Totowa, USA, p. 107-122

C. Haisch, K. Zell, J. Sperl, M. Vogel and R. Niessner; Quantitative Analysis with the Optoacoustic/Ultrasound System OPUS. Proc. of SPIE Vol. 7177 (2009) 717702-1-717702-9

N. Ivleva, M. Wagner, H. Horn, R. Niessner and C. Haisch; Towards Destructive Chemical Characterisation of Biofilm Matrix by Raman Microscopy. ABC 393 (2009) 197-206

X. Karsunke, R. Niessner and M. Seidel; Development of a Multichannel Flow-through Chemiluminescence Microarray for Parallel Calibration and Detection of Pathogenic Bacteria. Analytical and Bioanalytical Chemistry 395 (2009) 1623-1630

K. Kloth, R. Niessner and M. Seidel; A New Open Stand-alone Platform for Regenerable Automated Microarrays. Biosensensors and Bioelectronics 24 (2009) 2106.-2112

K. Kloth, M. Rye-Johnsen, A. Didier, R. Dietrich, E. Märtlbauer, R. Niessner and M. Seidel; A New Regenerable Immunochip for the Quick Determination of 13 Different Antibiotics in Raw Milk. Analyst 134 (2009) 1433-1439

M. Knauer, M. Carrara, D. Rothe, R. Niessner and N. Ivleva; Changes in Structure and Reactivity of Soot During Oxidation and Gasification by Oxygen, Studied by Raman Microscopy and Temperature Programmed Oxidation. Aerosol Science & Technology 43 (2009) 1-8

M. Knauer, M. Schuster, D. Su, R. Schlögl, R. Niessner and N. Ivleva Soot Structure and Reactivity Analysis by Raman Microspectroscopy, Temperature Programmed Oxidation and High Resolution Transmission Electron Microscopy. J. Phys. Chem. A 113 (2009) 13871-13880

D. Knopp, D. Tang and R. Niessner; Bioanalytical Applications of Biomolecule-doped Nanometer-sized Silica Particles. Anal. Chim. Acta 647 (2009) 14-30

C. Peskoller, R. Niessner, M. Seidel; Development of an Epoxy-based Monolith Used for the Bioseparation of Eschericha coli bacteria. J. of Chromatography A 1216 (2009) 3794-3801

C. Peskoller, R. Niessner and M. Seidel; Cross-flow Microfiltration System for Rapid Enrichment of Bacteria in Water. ABC 393 (2009) 399-404

M. Rieger, C. Cervino, J. Sauceda, R. Niessner and D. Knopp; A Highly Efficient Hybridoma Screening Technique Using Capture Antibody Based Microarrays. Anal. Chem. 81 (2009) 2373-2377

T. Schmid, U. Panne, R. Niessner and C. Haisch; Optical Absorption Measurements of Opaque Liquid Samples by Pulsed Laser Photoacoustic Spectroscopy. Anal. Chem. 81 (2009) 2403-2409

D. Tang, J. C. Sauceda, Z. Lin, S. Ott, E. Basova, I. Goryacheva, S. Biselli, J. Lin, R. Niessner, D. Knopp; Magnetic Nanogold Microspheres-based Lateral Flow Immunodipstick for Rapid Detection of Aflatoxin B2 in Food. Biosensors and Bioelectronics 25 (2009) 514-518

D. Tang, Z. Zhong, R. Niessner and D. Knopp; Double-codified Gold Nanolabels with Enhanced Electrochemical Immunoassay for Aflatoxin B1 in Food Using Multifunctional Magnetic Beads as Probes. Analyst 134 (2009) 1554-1560

D. Tang, R. Niessner and D. Knopp; Flow-injection Electrochemical Immunosensor for the Detection of Human IgG Based on Glucose Oxidase-derived Biomimetic Interface. Biosensors and Bioelectronics 24 (2009) 2125-2130

M. Wagner, N. Ivleva, C. Haisch, R. Niessner and H. Horn; Combined Use of Confocal Laser Scanning Microscopy (CLSM) and Raman Microscopy (RM): Investigations on EPS-Matrix. Water Res. 43 (2009) 63-67

2.2 Conference Presentations

2.2.1 Oral Presentations

C. Haisch, Photothermophoresis on Aerosols as a New Tool for Aerosol Characterization, International Conference on Photoacoustic and Photothermal Phenomena (ICPPP15), 19.-23.7.2009 Leuven, Belgien

C. Haisch, Innovative optische Methoden zum Biofilm-Monitoring, 3. Wasserseminar, 24.-25.6.09 Waidring, Österreich

C. Haisch, Photoakustik in der Analytischen Chemie, Seminarreihe des Forschungszentrums Jülich, 20.5.2009 Jülich

C. Haisch, Oberflächenverstärkte Raman-Spektroskopie als markierungsfreies Ausleseverfahren für Immuno-Mikroarrays, 6. Deutsches BioSensor Symposiums, 30.3.-1.4.09, Freiburg.

C. Helmbrecht, R. Niessner, Continuous Photophoretic Separation of Hydrocolloids, Euroanalysis 2009, 6.-10.9.2009, Innsbruck, Österreich

C. Helmbrecht, C. Haisch, R. Niessner, Photophorese: Eine neue Technik zur optischen Separation von Hydrokolloiden, Anakon 2009, 17.-20.3.2009, Berlin

C. Helmbrecht, R. Niessner: Photophoresis in a cross-flow setup – a new approach for the continuous separation of particular matter by optical forces, 19. Doktorandenseminar AK Separation Science, 11.-13.1.2009, Hohenroda.

N. P. Ivleva, M. Wagner, H. Horn, R. Niessner and C. Haisch, Chemical Analysis of Biofilm by Surface-Enhanced Raman Scattering (SERS), Wasser 2009, 18.-20.5.2009, Stralsund.

N. P. Ivleva, M. Wagner, H. Horn, R. Niessner and C. Haisch, Raman Microscopy and Surface-Enhanced Raman Scattering (SERS) for In Situ Analysis of Biofilm, FT-IR Spectroscopy in Microbiological and Medical Diagnostics 2009, 15.-16.10.2009, Berlin, Germany (invited)

D. Knopp; Antibodies as Molecular Tools for Bioanalytical Methods. Euroanalysis, 6.-10.9.2009, Innsbruck, Austria (invited).

D. Knopp; Environmental Immunoassays; 26.10.2009, University of Guelph, Canada.

D. Knopp; Immunoassays in Water Analysis. 60. Freiberger Forschungsforum 2009, Colloquium on Innovative Water Technologies. 17.-19.06.2009, Freiberg (invited).

D. Knopp; Transgenic Plants: A Valuable Alternative for Large-Scale Antibody Production and Phytoremediation. International Forum "Russia and Germany in the Common European Area. German-Russian Cooperation Network on Biotechnology", 11.-13.11.2009, Moscow, Russia (invited).

R. Niessner: Microarray-Technik in der Lebensmittelüberwachung. 7. Technologie-Formum Sensorik, Strategische Partnerschaft Sensorik, 29.6.2009, Regensburg (invited).

R. Niessner: Online Aerosol Characterization. Vienna Summer School "Basic Aerosol Science", 9.-10.7.2009, Vienna (invited).

R. Niessner: Microarray Technology – Status & Trends. Euroanalysis, 10.9.2009, Innsbruck (invited).

R. Niessner: Laboratory Investigation of Post-combustion Nitro-PAH Formation. Asian Aerosol Conference, 24.-27.11.2009, Bangkok.

R. Niessner: Photo-Thermophoresis as a New Tool for Aerosol Characterization. Asian Aerosol Conference, 24.-27.11.2009, Bangkok.

R. Niessner: Laser Light or Antibody – Two Friends to Analysts. FB Chemie, Univ. Ulm., 4.12.2009, Ulm (invited)

M. Schneider, A. Schubert, T. Baumann, F. Böhm, U. Steiner & C. Mayr, Vorstellung eines aktuellen Forschungsvorhabens zur hydrogeologischen Charakterisierung des Malms als tiefer Grundwasserleiter, Der Geothermiekongress 2009, 17.-19.11.2009, Bochum.

M. Seidel, S.C. Donhauser, A. Wolter, C. Peskoller, R. Niessner: Flow-Through Chemiluminescence DNA Microarrays for Multiplexed Quantification of Pathogenic Bacteria in Water. Euroanalysis 2009, 6.-10.9.2009, Innsbruck.

M. Seidel, S.C. Donhauser, G. Pappert, A. Nahrstedt, M. Heijnen, P. Paulicka, J. Überfeld, D. Sickert, M. Schienle, A. Frey, C. Stoll, A. Thiem, M. Bandilla, G. Hartwich, R. Niessner: Entwicklung instrumenteller Verfahren zur Anreicherung und Detektion multipler pathogener Keime im Trinkwasser. Wasser 2009, 18.-20.5.2009, Stralsund.

M. Seidel: Development of an Automated Microarray Chip Reader for the Multiplexed Analysis of Contaminants in Food and Water. Advances in Microarray Technology (AMT 2009), 19.-20.5.2009, Stockholm, Sweden (invited).

M. Seidel, A. Wolter, C. Peskoller, S.C. Donhauser, G. Pappert, R. Niessner: Kombination von Anreicherungstechniken und Analytischer Mikroarrays zur schnellen Detektion von pathogenen Keimen, Anakon 2009, 17.-20.3.2009, Berlin.

M. Seidel, A. Wolter, C. Peskoller, R. Niessner: Combining Rapid Enrichment Processes with Microarrays for the Detection of Multiple Pathogenic Bacteria in Drinking Water. enviroWater, 2.-4.3.2009, Stellenbosch, South Africa.

2.2.2 Poster Presentations

T. Baumann, L. Toops, C. Mayr & R. Niessner, Mobility Analysis of Nanoparticles and Hydrocolloids, Anakon 2009, 17.-20.3.2009, Berlin.

S. Donhauser, R. Niessner, M. Seidel: Schnelle und parallele Quantifizierung von E. coli, C. jejuni und L. pneumophila auf einem Chemilumineszenz-Mikroarray-Chip-Auslesegerät zur Trinkwasserüberwachung, Anakon 2009, 17.-20.3.2009, Berlin.

C. Helmbrecht, R. Niessner, Stability Evaluation of Nanometer-Sized Cu, Ag and Au Particles Using Asymmetrical Flow Field-Flow Fractionation (AF4), Euroanalysis 2009, 6.-10.9.2009, Innsbruck, Österreich

C. Helmbrecht, R. Niessner, Photophoresis – Separation of Hydrocolloids by Optical Forces, Wasser 2009, 18.-20.5.2009, Stralsund, Deutschland, Awarded Poster

C. Helmbrecht, R. Niessner, Calcium Carbonate: A New Standard for Particle Shape?, Anakon 2009, 17.-20.3.2009, Berlin.

G. Hörnig and R. Niessner, Analysis of Soot Deposition Mechanisms on the Gas Side Surface of Heat Exchangers used in Exhaust Gas Recirculation, Anakon 2009, 17.-20.3.2009, Berlin.

X. Karsunke, R. Niessner and D. Knopp; Mycotoxin Microarray for Food Monitoring. Anakon 2009, 17.-20.3.2009, Berlin.

K. Kloth, M. Rye-Johnsen, A. Didier, R. Dietrich, E. Märtlbauer, R. Niessner, M. Seidel: Development of an Open Stand-alone Platform (MCR3) – Rapid Determination of Antibiotics in Raw Milk, Anakon 2009, 17.-20.3.2009, Berlin.

M. Knauer, N. P. Ivleva, R. Niessner, C. Haisch, Surface-Enhanced Raman Scattering (SERS) as a Label-Free Readout Principle for Microorganisms on Microarray, FT-IR Workshop, 15.-16.10.2009, Berlin, Germany

C. Mayr, R. Niessner & T. Baumann, Schwefelwasserstoff im Tiefengrundwasser des Malmaquifers im Voralpenland, Geothermiekongress 2009, 17.-19.11.2009, Bochum.

C. Mayr, R. Niessner & T. Baumann, Gasförmiger Schwefel im Thermalwasser, Anakon 2009, 17.-20.3.2009, Berlin.

G. Pappert, R. Niessner, M. Seidel: Selektive Anreicherung von E.coli aus Wasserproben mittels Immunomagnetischer Separation, Anakon 2009, 17.-20.3.2009, Berlin.

C. Peskoller, R. Niessner, M. Seidel: Entwicklung von schnellen und selektiven Anreicherungsmethoden zur Probenvorbereitung von Mikroorganismen im Trinkwasser. Wasser 2009, 18.-20.5.2009, Stralsund.

M. Rieger, R. Plapperer, R. Niessner, M. Seidel: Entwicklung von Antikörper-gekoppelten Nanopartikeln als MRI-aktive Substanzen, Anakon 2009, 17.-20.3.2009, Berlin.

M. Rye-Johnsen, N. P. Ivleva, R. Niessner, C. Haisch, Surface Enhanced Raman Scattering as Readout Instrument for Microarrays, Anakon 2009, 17.-20.3.2009, Berlin.

M. Rye-Johnsen, N. P. Ivleva, R. Niessner, C. Haisch, Detection of Microorganisms in Water using a Raman-based Microarray Readout System, Wasser 2009, 18.-20.5.2009, Stralsund, Germany.

J.C. Sauceda, R. Niessner and D. Knopp; Mycotoxin Microarray for the Quantification of Ochratoxin A and Aflatoxins in Food Samples, Anakon 2009, 17.-20.3.2009, Berlin.

J.C. Sauceda, X. Karsunke, D. Knopp, and R. Niessner; Regenerable Microchip for Mycotoxin Determination in Food Samples. 6. Deutsches BioSensor Symposium, 30.3.-1.4.2009, Freiburg.

M. Seidel, S.C. Donhauser, K. Kloth, R. Niessner: Flow-through Chemiluminescence DNA Microarrays for Multiplexed Quantification of Pathogenic Bacteria. Medical Biofense Conference 2009, 20.-22.10.2009, München.

D. Tang, Y.L. Yu, Z. Lin, M. Miro, R. Niessner and D. Knopp; Magnetic Bead-based Bio-barcode Fluorescence Immunoassay for Aflatoxins in Food Using Biofunctionalized Silica Nanoparticles as Recognition Elements. Euroanalysis, 6.-10.9.2009, Innsbruck, Austria.

D. Tang, R. Niessner and D. Knopp; Synthesis of Micro- and Nanostructured Spherical Biocomposites using Sol-gel Technique, Anakon 2009, 17.-20.3.2009, Berlin.

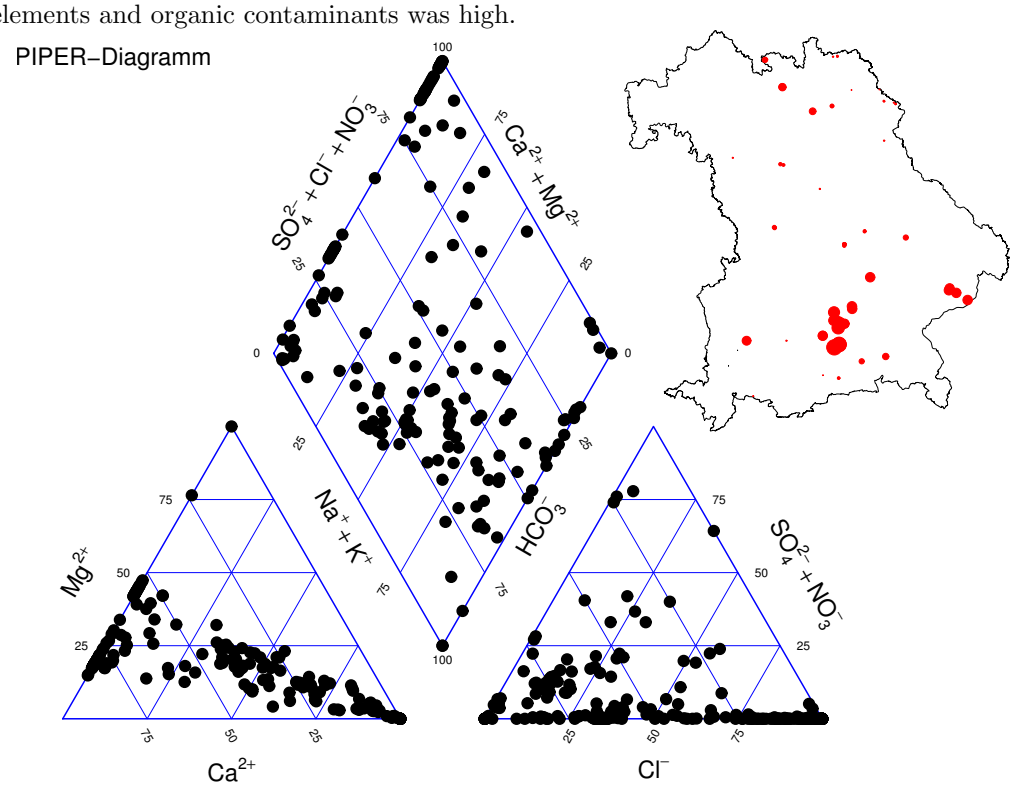
2.2.3 Organisation of Scientific Meetings

T. Baumann: Gordon Research Conference Flow & Transport in Permeable Media, 11.-17.7.2008, Oxford (Session Chair)

R. Niessner: 9. Dresdner Sensor-Symposium, 7.-9.12.2009, Dresden (Programme Committee)

2.3 Hydrogeological Consulting

The hydrochemical analyses in 2009 cover a large part of natural and contaminated groundwaters. The hydrochemical variability, both, with respect to the major ion ratios (see figure) and with regard to the concentration of major constituents, trace elements and organic contaminants was high.



Mineralisation control analyses Bad Abbach, Bayreuth, Bad Endorf, Bad Griesbach, Bad Gögging, Hölle, Kondrau, Künzing, Neumarkt i. d. Opf., Bad Rodach, Sibyllenbad, Straubing, Utting, Weißenstadt, Bad Wiessee, Bad Wimpfen, Bad Wörishofen

Hydrogeological and hydrochemical expertises (mineral water, spa water) Bad Abbach, Bad Gögging, Bad Füssing, Bad Staffelstein, Bitterfeld, Kondrau, Sibyllenbad, Treuchtlingen. Bad Tölz

Deep Hydrogeothermal Energy Exploration Altdorf, Aschheim, Dürrnhaar, Erding, Garching, Munich, Poing, Pullach, Sauerlach

2.4 Bachelor Theses

Peter Altenbuchner: Optimierung eines Chemilumineszenz-Mikroarrays zur Detektion von Mycotoxinen

Heide Bensch: Untersuchung von Nanopartikeln im Niederschlag und im Sickerwasser

Heinrich Birndorfer: Optimierung und Betrieb eines Prüfstandes zur Untersuchung von Rußablagerungen in Wärmetauschern der Abgasrückführung

Dominik Deyerling: Determination of the Content of Nitro-PAH in Real Diesel Soot Samples and in Artificially Pyrene-Coated Soot Exposed to NO_2 with HPLC

Tilman Flock: Development of a Label-free Readout Method for Microarrays

Ben Greisen: Optimierung eines Chemilumineszenz-Mikroarrays zur Detektion von Zearalenon

Christian Görner: Charakterisierung von $CaCO_3$-Partikeln mit Hilfe von FT-IR-Spektroskoskopie und Synthese von Standards

Ina Häuslein: Optimierung eines indirekt-kompetitiven Immunoassay zur Bestimmung von Aflatoxin B1 und Ochratoxin A in Erdnüssen am MCR 3

Claudia Hille: PAH- & NPAH-Analytik auf künstlichen Rußaerosolen

Maximilian Koch: Optimierung der Tetracyclin-Detektion in Rohmilch am MCR 3

Patrick Kotyla: Schwermetalltransport in einer mineralischen Basisabdichtung

Meera Annegret Mahle: Analyse von intakten polaren Lipiden in marinen Karbonatgesteinen

Franziska Mandl: Optimierung des Antibiotika-Nachweises in Milch/Honig am MCR 3

Lukas Pendzich: Laboruntersuchungen zur hydraulischen Leitfähigkeit von Verfüllmaterialien für Erdwärmesonden

Julia Pickelmann: Kolloide im Tiefengrundwasser

Stephanie Robu: Schnelle und parallele Quantifizierung von Salmonella typhimurium und Campylobacter jejuni auf einem Chemilumineszenz-Mikroarray-Chip-Auslesegerät

Patrizia Schöppner: Untersuchung der Lagerstabilität der Antibiotika-Mikroarray-Chips des MCR 3

Gabriella Somogyi: Hydrogeologie der Sauersbergquellen

Lisa Tröbs: Das Abbauverhalten von 3,6-Dichlorcarbazol in Böden

Aleksei Vjunov: Schnelle und parallele Quantifizierung von E.coli O157:H7 und L.pneumophila auf einem Chemilumineszenz-Mikroarray-Chip-Auslesegerät

Martina Weineisen: Optimization of the Regeneration Conditions for a Reusable Microarray Chip for the Detection of Ochratoxin A, Aflatoxin B1 and Aflatoxin B2

2.5 MSc and Diploma Theses

Cand. geol. Felix Grimmeisen: Die hydrogeologische Bedeutung der Mittelturon-Schichten innerhalb der Bodenwöhrer Senke

BSc Veronika Langer: Detection of E. coli – Specific Enzymes by Means of Antibody Microarrays

Cand. chem. Andreas Maier: Anreicherung von E. coli mittels monolithischer Affinitätschromatographie: Geometrie- und Anwendungsoptimierungen

Cand. geol. Manuel Moser: Combined Hydrochemical and Stable Isotope Study of the Aquifer System Campo Catragena (Murcia) in Southern Spain

BSc Lothar Opilik: Photophoretic Velocimetry for the Characterization of Aerosols

Cand.chem. Markus Oster: Kombination von Photophorese und Photoakustik

BSc Sonja Ott: Synthese und Charakterisierung eines Antikörper-Enzym-Konjugats für die immunologische Bestimmung von Aflatoxinen in Nahrungsmitteln

Cand. geol. Nicolas Peuckmann: Numerische Simulation des Strömungsfeldes und nicht reaktiver Stofftransportprozesse in einem künstlichen Aquifersystem

BSc Sandra Prell: Detektion und Quantifizierung von genmodifizierten Organismen mit Hilfe eines DNA-Microarrays

Cand. chem. Johannes Schmid: Charakterisierung der Reaktivität und Struktur von Dieselruß mittels Temperatur-programmierter Oxidation und Raman Mikroskopie

BSc Agathe Szkola: Optimierung von oberflächenverstärkter Raman-Spektroskopie (SERS) für die Analyse von Biomolekülen

2.6 PhD Theses

Apotheker Alexander Buhl: Entwicklung einer neuen Biosensor-Analysenmethode für die Diagnostik des Systemischen Lupus Erythematodes

Dipl.-Chem. Christian Cervino: Entwicklung von immunanalytischen, chromatographischen und massenspektrometrischen Methoden zur Bestimmung von Aflatoxinen in Lebensmitteln

Dipl.-Ing.(FH) Clemens Helmbrecht: Photophoretische Charakterisierung und Separation von Hydrokolloiden

Dipl.-Chem. Katrin Kloth: Entwicklung eines regenerierbaren Mikroarray-Chips zur simultanen Detektion von Antibiotika in Milch

Dipl.-Biol. Melanie Maier: Wirkung von verschiedenen Nanomaterialien auf das isolierte Herz von Meerschweinchen, isolierte Herzzellen und Neuronen

Dipl.-Phys. Tobias Roßteuscher: Online Monitoring of Biofilm in Microchannels with Thermal Lens Microscopy

Dipl.-Chem. Philipp Stolper: Entwicklung von online-Toxizitätstests für die wirkungsbezogene Analyse von Wasserinhaltsstoffen

MSc Zhe Sun: Synthesis and Application of Diclofenac Molecularly Imprinted Polymers for Selective Trace Analysis

Dipl.-Chem. Anne Wolter: Antikörper-Mikroarrays für die Analyse von Mikroorganismen im Trinkwasser

3 Teaching, Colloquia, and Other Activities

3.1 Classes

3.1.1 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

3.1.2 Chemical Engineering (Diplom)

- Aerosol Characterisation (Aerosolcharakterisierung); Niessner
- Environmental Measurement Technologies Lab (Praktikum Umweltmesstechik); Niessner, Haisch
- Gas Measurement Technologies/Chemical Sensors (Gasmesstechnik/Chemische Sensoren); Niessner

3.1.3 Pharmacy

- Instrumental Analytical Chemistry, (Instrumentelle Analytische Chemie); Haisch

  Lectureship at Ludwig-Maximilians-Universität München

3.1.4 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 Grundwasserschadensfällen); Baumann
- Technical Hydrogeology (Technische Hydrogeologie); Baumann
- Regional Hydrogeology (Regionale Hydrogeologie); Baumann
- Fluidflow in Porous Media Lab (Hydrogeologisches Laborpraktikum); Baumann, Haisch, Niessner
- Numerical Methods Lab (Hydrogeologische Modellierung II); Baumann
- Hydrogeological Field Lab (Hydrogeologische Feldmethoden); Baumann, Haisch

- Hydrogeological Mapping (Hydrogeologische Kartierung); Baumann, Haisch
- 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

3.1.5 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

3.1.6 ERASMUS Docent Mobility

- Immunoextraction and molecularly imprinted solid-phase extraction (MISPE); Master Course of Analytical Sample Preparation, (University of Palma, Mallorca, Spain) 30.03.-01.04.2009, Knopp

3.2 Institute Colloquia

Prof. Dr. Thomas Leisner, Forschungszentrum Karlsruhe und Universität Heidelberg: Cloud Processes Studies on Individual Levitated Droplets (12.1.2009)

PD Dr. Udo Weimar, Universität Tübingen: Gas Sensors: Principles and Applications (17.2.2009)

Dr. Alexander Makarov, Thermofisher, Bremen: Adventures of the Orbitrap Mass Analyser (25.2.2009)

Prof. Dr. Janina Kneipp, Humboldt-Universität Berlin: Surface-enhanced Raman Scattering for Bioanalytics (5.3.2009)

Dr. Maria-Magdalena Titirici, Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Golm/Potsdam: Smart Polymer Based Stationary Phases in Liquid Chromatography (12.3.2009)

Dr. Birgit Hülseweh, Wehrwissenschaftl. Institut für Schutztechnologien, Münster: DNA- and Protein Microarrays for the Fast and Sensitive Detection of Biological Warfare Agents (7.4.2009)

Prof. Dr. Hans Maurer, Saarland Univeersität Homburg/Saar: MS Approaches in Impaired Driving Toxicology (20.4.2009)

Prof. Dr. Peter Kämpfer: New Developments in Sampling and Identification of Airborne Microorganisms (28.4.2009)

Dr. Zeno von Guttenberg, OLYMPUS München: Microfluidic Applications of Surface Acoustic Wave Technology (19.5.2009)

Prof. Dr. Mario Thevis, Deutsche Sporthochschule Köln: Mass Spectrometry-based Detection of Drugs in Doping Controls (22.6.2009)

Dr. Liping Pang, Institute of Environmental Science and Research, Christchurch, New Zealand: "Hitching a Ride" – Bacteria-facilitated Migration of Cadmium and Colloid-associated Virus Transport in Groundwater (24.6.2009)

Dr. Petra Rösch, Friedrich-Schiller-Universität Jena: Raman-Spectroscopy as New Tool for Microorganism Detection and Characertization (13.7.2009)

Dr. Brigitte Dorner, Robert Koch-Institute, Berlin: Multiplexed Detection and Quantification of Microbial and Plant Toxins (30.7.2009)

PD Dr. Gerald Steiner, Technische Universität Dresden: Vibrational Spectroscopic Imaging of Cells and Tissue (14.9.2009)

Dr. Alexander Safatov, Vector State Research Center of Virology & Biotechnology, Koltsovo, Novosibirsk, Russia: Bioaerosols: Sources, Sinks and Measurements (15.9.2009)

Prof. Dr.-Ing. Jörg Müller, TU Hamburg-Harburg: PIMMS - A Planar Integrated Micro Mass Spectrometer (24.9.2009)

Prof. Dr. Andreas Thünemann, Bundesanstalt für Materialforschung und –prüfung, Berlin: Characterization of Polymers & Nanoparticles by Online Coupling of Field-Flow Fractionation with SAXS and other Detection Principles (9.11.2009)

Dr. Nico Goldscheider, Centre of Hydrogeology, University of Neuchâtel/Schweiz: Continuous Monitoring of Particle-Size-Distribution as an Early-warning System for Microbial Contamination of Karst Groundwater (19.11.2009)

Prof. Dr. Diethelm Johannsmann, Clausthal University of Technology: What can the Quartz Crystal Microbalance Tell us about Complex Soft Samples? (20.11.2009)

3.3 External Tasks and Memberships

Prof. Dr. Reinhard Niessner

German Council of Science & Humanities, External Evaluation Comittee	Member (4/2010)
Evaluation Committee for Antwerp Analytical Chemistry	Member (4/2010)
Bayer. Fachausschuss für Kurorte, Erholungsorte und Heilbrunnen	Member
DECHEMA Commission "Chemische Grundlagen und Anwendungen der Sensortechnik"	Member
DFG-Senatskommission für Wasserforschung	Member (until 3/2009)
Heinrich-Emanuel-Merck-Award Committee	Jury Head
Analytical Chemistry	Associated Editor
Analytical and Bioanalytical Chemistry	Advisory Board Member
Microchimica Acta	Advisory Board Member
Fresenius' Environmental Bulletin	Advisory Board Member
Analytical Sciences	Advisory Board Member

PD Dr. Thomas Baumann

Bayer. Fachausschuss für Kurorte, Erholungsorte und Heilbrunnen	Member
VBEW AK Grundwasserschutz	Member
DIN NA 119-01-02-05 UA Elution	Member

Prof. Dr. Dietmar Knopp

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

Dr. Michael Seidel

KRdL-3/7/04, "Luftgetragene Mikroorganismen und Viren", im VDI/DIN	Member
DECHEMA ad hoc Arbeitsgruppe Biosicherheit	Chair

4 Equipment

4.1 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.

Additionally three landfill monitoring sites, one municipal solid waste landfill, one MSWI bottom ash landfill, and one mixed waste landfill are run by the institute.

4.2 Environmental Analytical Chemistry

4.2.1 Dioxin Laboratory

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

4.2.2 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)

4.2.3 Bioanalytics

Bioseparation:
Crossflow Filter (Inge AG)
Crossflow Filter (Spectrum Laboratories, Inc)
Pressure and Flowrate controlled Crossflow Filtration System (IWC)
Molecular Biology:
1 Biacore X100, General Electric
1 Real-time PCR (Light Cycler 480, Roche) Microarray Technology:
3 Chemiluminescence Microarray Reader (PASA, IWC)
2 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 (Haerasafe KS, Kendro)
1 Microbiological Incubator (BD 53, Binder)
1 Autoclave (Century 2100, Prestige Medical)
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

4.2.4 Chromatography and Particle Separation

3 GCs with FID, NPD, ECD, TEA, and AED
1 Orbitrap-based benchtop MS, Exactive/HCD-System, Thermo Fischer
1 High-resolution GC/MS, VG Autospec
1 Asymmetrical Field-flow-fractionation system
1 SFE-System with modifier, Suprex
2 Concentrators for dynamic headspace analysis
1 High-speed counter-current-distribution chromatographie system

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

4.2.5 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

4.2.6 Laser

3 He/Ne-laser
6 Nd-YAG-laser
1 CO_2-laser
3 Dye-laser (tuneable 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
1 Optical parameter oscillator (410 nm - 2.1 μm)

4.2.7 Optoelectronics/Spectrometer

1 Rowland spectrometer
2 Echelle spectrometer
1 FTIR-Spectrometer, Perkin Elmer 1600
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 Boxcar integrator
4 Digital storage oscilloscopes (400 MHz, 500 MHz)
3 Optical multichannel analysators with monochromators, time-resolving
3 Intensified CCD cameras
1 Wavemeter

4.2.8 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 nm, 633 nm, 780 nm)

4.2.9 Sum Parameters

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

5 Staff 2009

Univ.-Prof. Dr. Reinhard Niessner

PD Dr. Thomas Baumann
Dr. Christoph Haisch
Dr. Clemens Helmbrecht (from 10/2009)
Dr. Natalia P. Ivleva
Dr. Kathrin Kloth
Prof. Dr. Dietmar Knopp
Dr. Michael Seidel

Birgit Apel
Christine Beese
Julius El Masry
Roswitha Glunz
Joachim Langer
Susanne Mahler
Christine Sternkopf
Christa Stopp
Sebastian Wiesemann

Hatice Hazir
Mira Kolar

PhD Students

MSc Chem. Matteo Carrara
MSc Chem. Simon Donhauser
Dipl.-Ing. Clemens Helmbrecht (until 10/2009)
Dipl.-Ing. Gabriele Hörnig
Dipl.-Ing. Susanne Huckele
Dipl.-Chem. Xaver Karsunke
Dipl.-Chem. Markus Knauer (until 9/09)
MSc Veronika Langer
MSc XiangJiang Liu
Dipl.-Geol. Christina Mayr
MSc Sonja Ott
Dipl.-Biotechn. Gerhard Pappert
Dipl.-Chem. Caroline Peskoller (until 8/09)
MSc Sandra Prell (from 2/09)
MSc Chem. Martin Rieger
MSc Chem. Maria Knauer
MSc Chem. Jimena Sauceda
Dipl.-Chem. Johannes Schmid
MSc Agathe Szkola (from 2/09)

External PhD Students

Apotheker Alexander Buhl (Klin. re. d. Isar) (until 4/09)
Dipl.-Biol. Melanie Maier (GSF) (until 12/2009)
Dipl.-Phys. Peter Menzenbach (INNOLAS, Krailling)
Apothekerin Carolin Müller (Klin. r. d. Isar)
Dipl.-Chem. Tobias Roßteuscher (z.Zt. Prof. Kitamori, Tokyo, until 6/09)

Diploma Students/MSc Students

cand. geol. Felix Grimmeisen (4/09-10/09)
BSc Uta Jäger (until 8/09)
cand. geol. Manuel Moser (4/09-10/09)
BSc Andreas Maier (2/09 bis 7/09)
BSc Lothar Opilik (1/09 bis 6/09)
cand. chem. Marcus Oster (until 5/09)
cand. chem. Schaller, Andreas (5/09 bis 10/09)
MSc Jan-Christoph Wolf (from 3/09)
MSc Klaus Wutz (from 4/09)

Guests and Research Fellows

MSc Evgenia Basova, Saratov University, Russia (until 3/09)
Dr. Anne Johansen, Central Washington University (until 8/09)
Dr. Dianping Tang, University Chogqing (until 9/09)
Dr. Martin Gonzales, Ingenieria Universidad de Buenos Aires (from 4/09)
MSc Zhen Lin, TsingHua University (6/09 bis 9/09)
Dr. Irena Goryacheva, Saratov University (9/09 bis 10/09)
Dr. Piyada Songsermsakul, Khon Kaen University, Thailand (9/09 bis 10/09)
MSc Natalia Beloglazova (from 10/09)
MSc Anna Proydakova (from 10/09)

Student Assistants

Christine Acher (4/09 bis 10/09)
Heinrich Birndorfer (from 11/09)
Christian Görner (3/09 bis 9/09)
Marco Kerl (5/09 bis 7/09)
Maximilian Reitzel (until 5/09)
Martina Ueckert (until 5/09)
Sebastian Weiker (from 12/09)