



Institute of Hydrochemistry

Chair for Analytical Chemistry

Annual Report

2006

The main title of the report is centered on the page. It is composed of four lines of text, all in a bold, black, sans-serif font. The first line is 'Institute of Hydrochemistry', the second is 'Chair for Analytical Chemistry', the third is 'Annual Report', and the fourth is '2006'.

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Chair for Analytical Chemistry
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Marchioninstr. 17

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Editor: Dr. Thomas Baumann

Editorial

Dear coworkers, friends and colleagues,

it is my personal pleasure to present another issue of our annual report. I hope you will enjoy reading about our research activities.

Last year has seen a number of momentous events and decisions, both, on a political and a scientific level. To begin with, TUM's application in the first round of the "Excellence Initiative" was successful and TUM, as one of three top-level research institutions in Germany, received extra funding to continue its research excellence. We are accepting this as an incentive to maintain and improve our research and teaching activities.

The trend towards higher student numbers is continuing. This year we are expecting several hundred Freshmen in a new programme called "Environmental Engineering Technology". In chemistry, chemical engineering and geological sciences, we expect an increase of 40% on average. After several years of having hardly enough students to run the research projects, it seems that we will soon be overrun, and not only in lab classes. In addition, tuition fees will raise expectations in the quality of teaching and supporting materials.

The year 2006 brought another significant change to the institute's internal structure and research focus: PD Dr. Weller received a call to the Berlin Federal Institute for Material Research. There, he is founding director for a new bioanalytic section, focussing on the standardization and reliability of bioanalytic techniques.

On the other hand, I am pleased to announce that two senior scientists, Dr. Pöschl and Dr. Baumann have received their habilitation degree. These two scientific success stories, in the fields of aerosol chemistry and physics and hydrogeology, underline the institute's lively, multi- and interdisciplinary research. Also the Microarray Group, started a year ago, and is making good progress. We are expecting a first protein chip, spiked with antibodies for microorganism detection, soon.

Another modification passed almost unnoticed, the Institute of Hydrochemistry now hosts the Chair for Analytical Chemistry. Looking at the research areas covered by the different groups, including automotive, medical and environmental applications, this new name is a common denominator and better reflects the Institute's scientific mission.

The perspective for 2007 is encouraging. Many research proposals have been submitted and, although the competition is high, I am confident that we are addressing research topics of general interest.

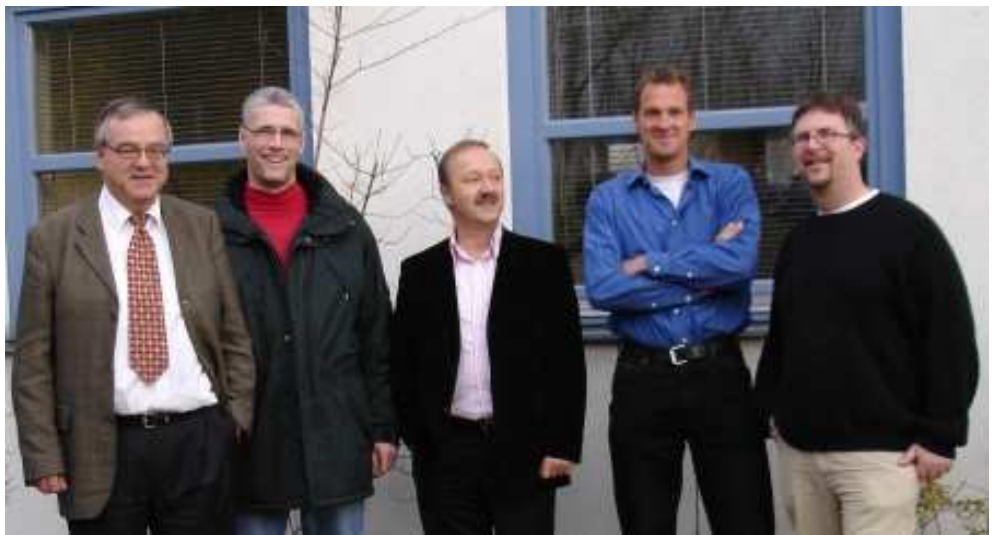
Finally, I'm very grateful for the efforts of all the institute's members. I would also like to thank the various funding institutions, and especially our "Freundeskreis" for preserving our freedom of research through their financial contributions.

All the best for the year 2007!



Reinhard Nießner
Head of the Institute

Head of the Institute and Group Leaders 2006



R. Niessner, T. Baumann, D. Knopp, C. Haisch, M. Seidel

1 Research

1.1 Hydrogeology and Hydrochemistry

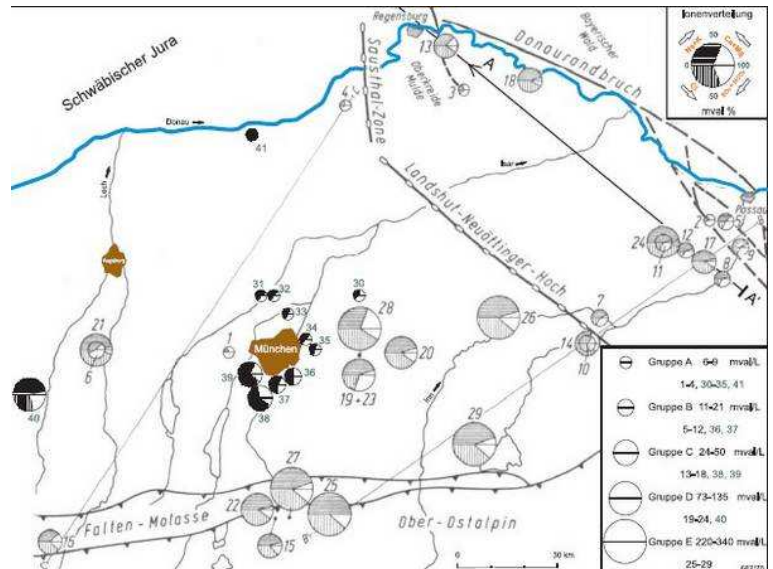
1.1.1 Hydrochemistry of the Malm Aquifer

Funding: Private Enterprises

During recent years a number of wells exploring the Malm aquifer have been installed in the vicinity of Munich. These groundwater wells are used for geothermal energy production. With the availability of new data on the chemical composition of the groundwater in the Malm aquifer, previous hypothesis on the hydraulic and hydrochemical conditions can be put to the test. Currently all geothermal energy projects have been designed as doublet systems with a production well and a reinjection well, which receives the water after it has been cooled down. Detailed knowledge is needed to predict the long term performance and environmental effects of the geothermal energy projects.

In cooperation with our partners, we collected and edited data from all major geothermal energy projects in the vicinity of Munich. Additional data from the East Bavarian region was collected for comparison. In the first phase of the project the focus was on the main chemical constituents of the groundwater. Isotopes and trace elements will follow.

(*R. Hentschel, T. Baumann*)



1.1.2 Colloid Transport in Multiphase Systems

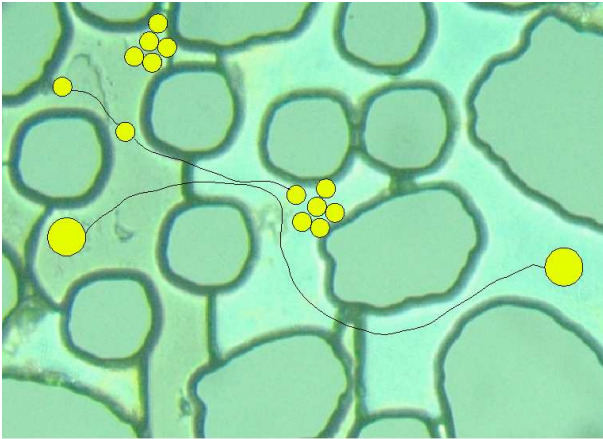
Funding: DFG Ba 1592/3-1

Understanding colloid transport is necessary to better comprehend contaminant infiltration into aquifers, to protect water used domestically, and/or to properly manage and remediate environmental contaminants. In the past, the problem with studying colloids in situ or with a column test was that it was difficult to access what was actually happening on the pore scale (e.g., particle-particle interactions and interactions at (reactive) interfaces). Micromodels designed to replicate porous media and allowing visual access to the pore space have been and are used to gain data and information about the processes in porous media. Micromodels also allow for microscopic analysis of fluid flow and permit visualisation and quantification of colloid transport and filtration.

In the past, micromodels have been used for quantifying dispersion of *E. coli*, observing the dissolution of non-aqueous phase liquids (NAPLs), and studying the behavior of colloids at different interfaces. For this project, micromodels are used to visualise and quantify colloid diffusion and dispersion in a porous environment. In addition, this project is using a new approach to quantifying pore-scale transport mechanisms of colloids using particle image velocimetry (PIV). PIV uses pattern matching to identify

particle movement and velocity from a series of video images. In an industrial context, PIV is used to quantify air flow or fluid flow in systems too complex to simulate, that is the particles are used as inert tracers. In our case, the particles (colloids) themselves are in the focus of research.

Colloid transport experiments are usually evaluated manually, meaning that the trajectories for each colloid are derived from a series of images. Although manual tracking has high reproducibility, counting particles by hand is very time consuming and operator dependant. Therefore, PIV could be a possibility to provide the same information that manual tracking provides (e.g., number of particles, particle direction, and particle velocity), yet provide this information in a more timely manner.



Colloid diffusion and dispersion were examined on a single-particle level through digital imaging with a CCD camera for multiple images per second and single images using a SLR camera. The experiments used fluorescent latex colloids with various sizes in a micromodel with heterogeneous pore geometry. Flow was established using a hydraulic gradient setup at varying flow rates. MatPIV, an extension to Matlab, was used for the PIV evaluation.

Imaging results show that colloids do diffuse into the porous media, but not as extensively as a molecule. This is understandable due to the difference of colloid size and mass to that of a small molecule. With each experiment several different colloid sizes were compared to see if there were differences in diffusion, and if colloid concentration, flow velocity of the environment, and ionic strength had an influence on colloid diffusion as well. Experiments were under continuous flow conditions in a completely saturated environment.

For theoretical evaluation of colloid diffusion and dispersion, some of the micromodel velocity fields calculated with a Lattice Boltzmann (LB) model were available and were used together with a particle transport model to validate the results of PIV. Diffusion effects and theoretical simulations to assess the limits of detection and the accuracy in micromodel experiments were based on Random Walk models.

(L. Toops, T. Baumann)

1.2 Bioanalytics

1.2.1 Development of Rapid Multidimensional Immunoanalytical Methods for Detection of Mycotoxins in Foods and Feeds

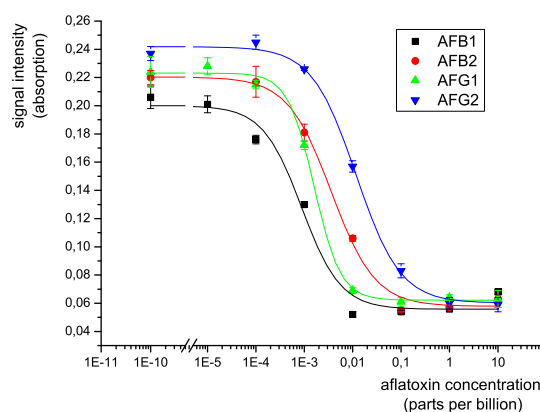
Funding: IWC

Mycotoxins are toxic secondary metabolites produced by several species of fungi on agricultural commodities in the field or during storage. Among them, aflatoxins are of ongoing concern due to their high carcinogenicity. Four structurally related aflatoxins (aflatoxins B1, B2, G1, and G2) naturally occur and are of interest for many foods/feeds. Conventional routine instrumental analysis is presently very time and labor intensive, since the maximum permissible limits given by law are low (μg per kg range and below) and the matrices are usually complicated (e.g. alcoholic extracts of peanuts or coffee). Thus, there is a strong demand for rapid and reliable analytical screening methods. This project is dedicated to the development of automatized immunoanalytical methods to provide a solution to these problems.

Within the project, aflatoxin selective antibodies are presently generated. Various aflatoxin-derived haptens and protein conjugates have been chemically synthesized, e.g. for use as immunogens. The figure on the right contains calibration curves of an aflatoxin-selective antibody, which shows certain cross-reactivities to the four aflatoxins of interest. The project includes the generation of three more aflatoxin selective monoclonal antibodies that show differing cross-reactivity patterns. By means of such antibodies, a multidimensional immunoanalytical method, i.e. an antibody-based method for measurement of real samples containing mixtures of the four aflatoxins, will be possible.

The project furthermore addresses the development of a regenerative mycotoxin biochip on which the toxins will directly be immobilized. Our in-house developed microarray chemoluminescence reader provides the analytical platform. The automatized immunoanalytical method will enhance the analytical accuracy and reproducibility and will dramatically reduce the time required for one analysis. The system will be designed for application in routine food analysis and will, therefore, be of particular interest for analytical laboratories, food producers, traders and the food processing industry.

(C. Cervino, D. Knopp)



1.2.2 Effect-Directed Analysis of Toxins by LC-MS Coupled With Online Toxicity Tests

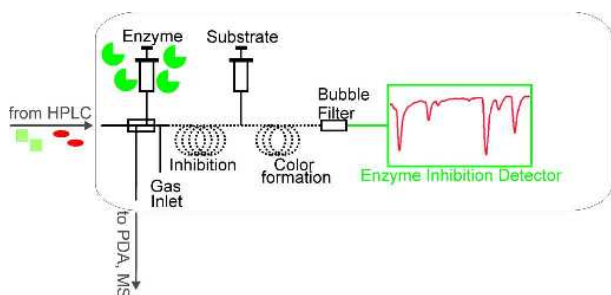
Funding: BMBF 02WU0331

Cooperation: Institute of Technical Biochemistry (Stuttgart), Helmholtz Centre for Infection Research (Braunschweig)

The identification of biological active compounds in complex matrices, such as environmental samples, is often desirable, especially in the field of water surveillance. For environmental monitoring it is important to have a tool at hand that helps to focus on relevant substances and does not provide a flood of information. By using a simple toxicity test, one often gets sum parameters without getting the source of the toxic

effect. Therefore, chemical analysis is an important step in water monitoring to get chemical information. Other requirements to a system used for monitoring are easy handling and fast analysis. Effect-directed analysis, which combines physicochemical separation and chemical analysis with a biomolecular recognition step, is a useful approach in this direction.

In this work, a system in terms of effect-directed analysis is set up to combine high performance liquid chromatography (HPLC) with a photodiode array, a mass detector and a biochemical detector. For testing neurotoxic effects, an acetylcholine esterase based detection system is used. To gather general toxic information, another system based on the toxicity test with *Vibrio fischeri* is used. Water samples spiked with different pesticides and phenols is separated by chromatography on a C18 column.



After the separation column, the flow is split in three streams. One leads to the photodiode array to gather information about absorbance properties depending on wavelength. Via the second flow path, the analytes flow to an electrospray ionisation - time of flight mass spectrometer to gain information about molecular mass or structural

information by fragmentation. The last flow path leads into the biodetector. An online enzyme inhibition assay, based on acetylcholine esterase, was used. The detector included an online enzyme inhibition reactor, followed by a colour forming step using acetoxy-methyl-quinolinium iodide. The detection of the dye was performed with a fluorescence detector (figure).

To preserve the separation achieved in the HPLC, air bubbles are introduced in the biodetection system to obtain small compartments of the liquid phase. Another advantage is the increased mixing within one segment. Thus the band broadening is almost nonexistent.

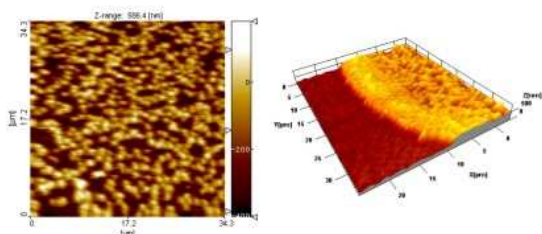
(P. Stolper, D. Knopp, M. Weller)

1.2.3 Biomimetic Optical Sensors for Environmental Endocrine Disruptor Screening (MENDOS)

Funding: EU (QLK-4-CT2002-02323)

During the last few years, endocrine disrupting chemicals (EDCs) have become suspects in various reproductive anomalies in humans and wildlife, mimicking the behaviour of estrogen and other endogeneous hormones. Following the large number of chemicals with potential endocrine effects, screening methods should be capable of detecting many classes of compounds in a reasonable short time and offer the possibility of on-site analysis to identify contamination in rivers, industrial effluents, sewage water, and water resources used for drinking water. The main aim of the EU project MENDOS was the development of novel artificial receptor based optical sensor systems.

This subproject focussed on the synthesis of molecularly imprinted polymers (MIPs) for polycyclic aromatic hydrocarbons and phthalic acid compounds. Both chemicals constitute highly lipophilic compounds without any pronounced functional groups in their molecules. Imprinting is difficult because the usual non-covalent interactions



like hydrogen bonds, dipolar and/or ionic interactions cannot be formed. The only interactions that can be employed in the imprinting and recognition process are the hydrophobic interaction, steric cavity, and pi-pi interaction, which are one or two orders of magnitude weaker than the electrostatic forces.

Different methods, such as bulk polymerization (BP), precipitation polymerization (PP) and mini-emulsion polymerization (MEP) were used and the characteristics of the particles investigated. The polymers were used for several applications such as SPE support, chromatographic stationary phase, and recognizing layer on sensor surfaces (Figure: AFM images of DEHP MIPs spotted on a glass chip (in Collaboration with Dr. Claudia Preininger, ARC Seibersdorf, Austria, Dr. Levy Gheber, Ben Gurion University Beer-Sheva, Israel, Prof. Karsten Haupt and Dr. Anne-Sophie Belmont, Compiègne University of Technology, France).

(M. Yang, D. Knopp)

1.3 Applied Laser Spectroscopy

1.3.1 Non-Destructive Analysis of Biofilm Matrix by Raman Microscopy

Funding: DFG

Cooperation: Prof. Horn, TUM

Biofilms are complex structures growing on nearly every surface that is in contact with water. In addition to cellular constituents, the second most important fraction in biofilms are extracellular polymeric substances (EPS). For in situ assessment of the biofilm structure, the confocal laser scanning microscopy has been proved to be a powerful technique. However, for distinction of different species staining is necessary,

although not ideal. Moreover, the staining of the total EPS is difficult because EPS are a mixture of different polymers including polysaccharides, proteins, nucleic acids, and amphiphilic polymers.

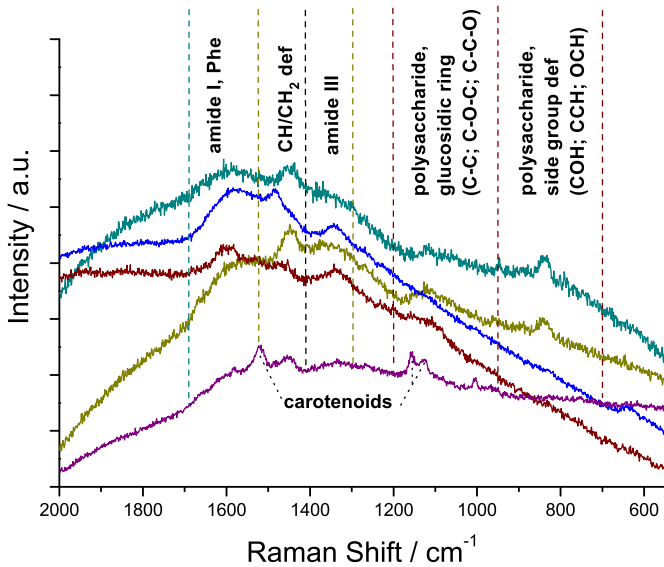
We expect that Raman microscopy helps to overcome these limitations and provides more detailed information about biofilm composition. Raman spectroscopy is based on inelastic light scattering and provides fingerprint spectra. It requires no or little sample preparation, and Raman spectra can be obtained non-invasively without staining and influence of water. Moreover, the coupling of Raman spectroscopy with microscopy (Raman Microscopy) enables high spatial resolution (laser beam diameters as small as $\approx 1 \mu\text{m}$) and sensitivity.

We analyzed the Raman spectra of a wide range of reference compounds that can be present in biofilms (polysaccharides, proteins) and found significant differences in the “fingerprint” region. The biofilm-specific

polysaccharides (dextran, xanthan, gellan and alginate) show bands of various forms and intensities in three major regions: CH/CH₂ def., 1500-1200 cm⁻¹; ring mode region, 1200-950 cm⁻¹; and side-group def., 950-700 cm⁻¹. These differences can be used for identification of individual components in EPS.

Spectra from different parts of biofilm, obtained at 514 nm, exhibit a strong fluorescence background. But the spectra obtained at 633 nm contain multiple bands (due to biofilm components such as polysaccharides, proteins and carotenoids) and provide more detailed information about the composition of the biofilm matrix (see Figure). Our results indicate that Raman microscopy is a promising tool for the analysis of biofilms.

(N. Ivleva, C. Haisch)

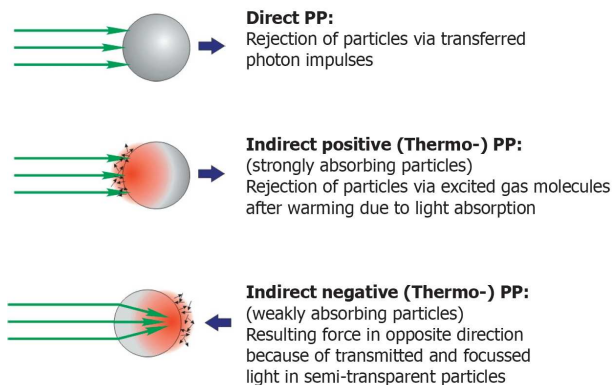


1.3.2 Photophoretic Particle Separation

Funding: DFG

Photophoresis (PP) denotes the phenomenon that small particles suspended in gas (aerosols) or liquid (colloids) start migrating when illuminated by an intense beam of light. In case the particle is transparent and the index of refraction is larger compared to the surrounding medium, the particle moves in a forward direction away from the light source, due to the momentum transfer from the photons. Interestingly, motion can occur in the direction of light (positive PP) and in the opposite direction (negative PP) as well. If the particle absorbs the incident light, a temperature gradient can be developed which causes the migration according to its thermal and optical properties and is termed Thermo-PP.

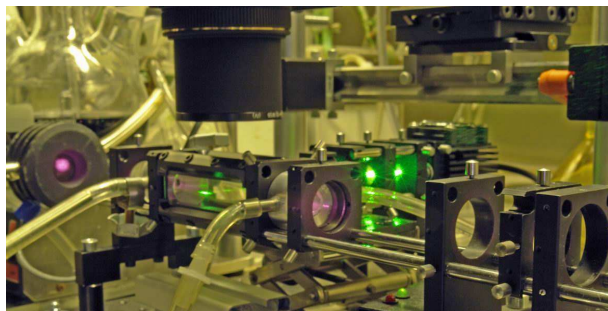
In conventional separation techniques, aerosols and colloids are separated by means of electrical, thermal or flow fields. Funded by the DFG, the application of light is tested as a possibility of separating particles due to their optical properties. Such a separation technique would allow, e.g. the isolation of organic from inorganic particles of the same size.



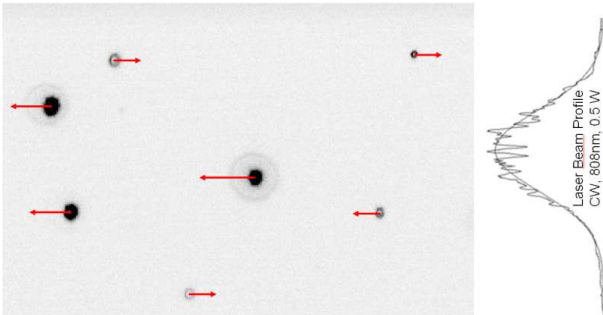
Photophoresis on Aerosols We aim to develop a continuous flow separation system for aerosols regarding the optical properties of the particles. Hence, we started with a first setup to characterize direct PP and indirect (thermo) PP by using particles of different size and optical properties. The experiments take place in a flow cell with a rectangular cross section positioned horizontally or vertically at normal pressure conditions.

The particles in the flow cell move from the left to the right, forced by a constant air flow stream. A diode laser, directed against the flow, is used to slow down the particle velocities, hold the particles at a certain position or move the particles against the flow by means of photophoretic force. The migration of the single particles is observed by a CCD camera and monitored by a computer. From an image series, the PP velocities of the single particles are obtained by particle imaging velocimetry, based on pattern matching on two sequential frames.

Experiments with polystyrene latices ($0.5 \mu\text{m} - 1.9 \mu\text{m}$) verify the linear correlation between the particle size and the measured PP velocities. The highest PP velocities were found for monodisperse soot particles with a very low thermal conductivity and therefore a high temperature gradient within the particle. Future experiments will be dedicated to investigate the influence of particle size and difference in materials simultaneously.



Photophoresis on Colloids The photophoretic force, acting on particles suspended in water, is generated by a HeNe laser which provides power up to 45 mW at a wavelength of 632.8 nm. The laser beam is focussed by a lens ($f'=40$ mm) onto the particles in the middle of a flow cell. Knowing the frame rate of the recording camera, the photophoretic velocity from single particles are calculated from the digital images by a PIV algorithm.



The velocities of latex particles of different diameters, 1.90 μm , 2.88 μm , 4.13 μm and 5.09 μm respectively, were measured at different laser powers. As predicted by theory, the photophoretic velocity is directly linear to the laser power for the particle sizes and energies used in this work. Besides Latex micro-particles, Melamine, and Monosphere (SiO_2), particles with a particle diameter of $\approx 1 \mu\text{m}$, were characterized by their photophoretic behaviour of transparent particles .

By determination of single particle velocities in a known light intensity distribution, laser photophoresis could open up the possibility for the identification and characterization of particles due to the differences in their optical and thermal properties. Moreover, this fact could be used for separation of inorganic particles, bacteria or living cells of the same size, but different properties or shapes. The application of photophoretic forces is a promising technique for characterization and separation, and is a gentle and touch-free technique for sensitive samples. (C. Helmbrecht, C. Kykal, C. Haisch)

1.3.3 OPUS - Optoacoustics in Combination with Ultrasound for Breast Cancer Detection

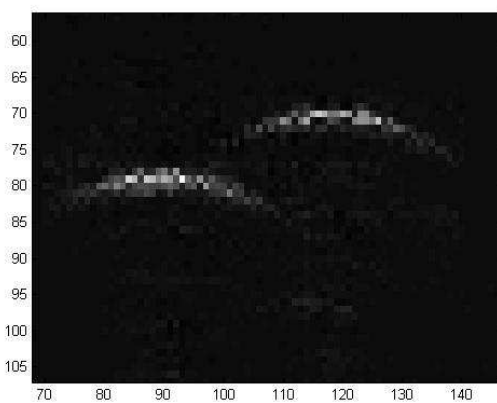
Funding: Bayerisches Staatsministerium für Wirtschaft, Infrastruktur, Verkehr und Technologie, Program: BayMed

Cooperation: General Electric, München; InnoLas, München

The most commonly used methods for breast cancer detection are mammography and sonography. In contrast to sonography, mammography is associated with radiation exposure. Depending on the properties of a patient's breast, mammography and sonography can not always be used. Ultrasound imaging is based on acoustical properties of tissue, or more precisely on their reflection of the sound wave. The acoustical properties of different tissues show only a slight variation which makes them difficult to distinguish. However, they show specific variations in their optical properties.

In photoacoustics, the ultrasound wave is induced by nanosecond laser pulses. The light becomes absorbed in the media and causes a local heating, which is followed by an adiabatic extension and a pressure wave. The amplitude of the ultrasound wave therefore depends on the absorption of the sample. A combination of photoacoustics with ultrasound would result in an improved contrast in the acoustic output.

The goal of this project is to couple a photoacoustical system to a conventional sonograph, combining the high contrast of photoacoustics with the spatial resolution of



conventional ultrasound systems. The main steps for this combination are the trigger set-up and the coupling of light into the tissue below the ultrasound head with homogeneous intensity distribution. A special challenge is the required compliance with the standards for medical equipment. Another focal point lies in the development of a tissue phantom to test the system. Phantoms intended for use in photoacoustics must possess both optical and acoustical properties of tissue. Therefore, these properties of tissue had to be investigated.

Photoacoustic experiments with the combined system on simplified phantoms have been performed successfully, as shown in the above figure, which shows the photoacoustic image of two absorbing rods ($D = 3 \text{ mm}$) embedded in a tissue phantom.

(K. Zell, C. Haisch)

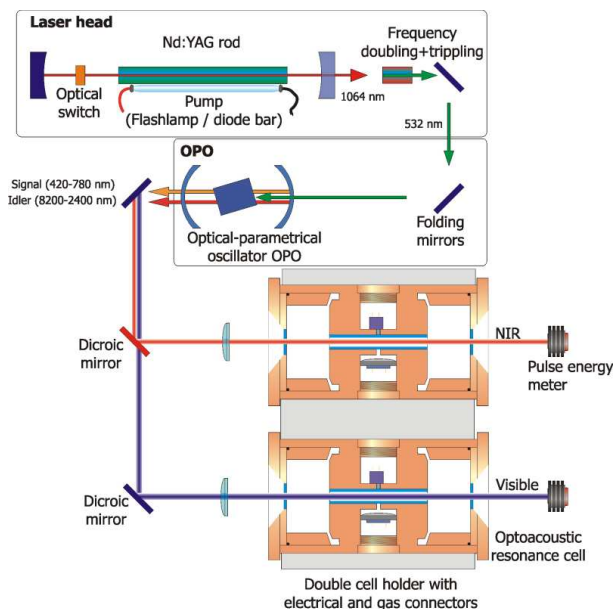
1.3.4 Combination of Cavity Ring Down Spectroscopy (CRDS) with Photoacoustical Detection Methods to Determine the Optical Properties of Aerosols

Funding: IWC

The goal of the project is the design of an optoacoustical device to measure complete absorption spectra of aerosols in the UV, Vis and NIR spectral range. One application of such instrument can be the distinction between organic and inorganic aerosols. In contrast to other photoacoustic measuring systems developed at the IWC, the new system will work with a pulsed laser source, which allows the application of small-scale Nd-YAG-laser in combination with an OPO. With this tool, the complete spectral range desired should be amenable with a robust, compact and even transportable instrument, offering high sensitivity and a wide dynamic range. A schematic drawing of the planned set-up is shown in the figure.

The next step, will be the further improvement of the sensitivity, which will be achieved by combining photoacoustics with the Cavity Ring Down Spectroscopy method (CRDS) in a single cavity.

(P. Menzenbach, C. Haisch)



1.4 Nanoparticle Research

1.4.1 Raman Microspectroscopic Analysis of Size-Resolved Atmospheric Aerosol Particle Samples

Funding: BMBF, AFO2000 Project 07ATC05, CARBAERO

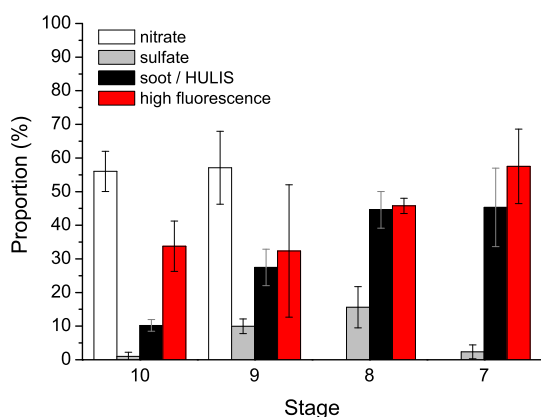
Aerosols are of great importance for atmospheric chemistry and physics, the climate, and public health. Among the predominant chemical components determining the properties and effects of air particulate matter are sulfates, nitrates, sea salt, organic compounds, and so-called black or elemental carbon.

Raman spectroscopy provides fingerprint spectra that allow the distinction of a wide range of chemical substances, including soot, related carbonaceous materials, and inorganic salts in aerosol samples. Raman microspectroscopy (RM), which combines the analytical capabilities of Raman spectroscopy with the spatial resolution of an optical microscope, enables investigation of individual aerosol particles.

We apply RM and Raman mapping for the analysis of soot, humic-like substances (HULIS) and inorganic compounds in size-resolved samples of air particulate matter, collected with an electrical low-pressure impactor (ELPI). The spectra of soot particles from different ELPI stages were fitted with a combination of four Lorentzian-shaped bands (G, D1, D2, D4 at about 1580, 1350, 1620, and 1200 cm^{-1} , respectively) and one Gaussian-shaped band (D3 at about 1500 cm^{-1}). The ELPI samples of sub-micrometer atmospheric particles exhibited essentially the same Raman spectra and parameters as standard diesel soot. In winter samples, this was also the case for larger particles with aerodynamic diameters up to 4 μm . Spring and autumn samples, however, exhibited increased D1 band widths and D3 band intensities, indicating a high prevalence of HULIS in the size range of 2-4 μm .

In addition, various nitrates and sulfates (mostly NaNO_3 and $(\text{NH}_4)_2\text{SO}_4$; some NH_4NO_3 , $\text{Ca}(\text{NO}_3)_2$, Na_2SO_4 , and CaSO_4) and small amounts of CaCO_3 were detected. Single- and multi-component spectra indicated the presence of both externally and internally mixed particles. The relative abundance of different chemical components in different particle size ranges was quantified in mapping experiments (0-55% NaNO_3 , 1-15% $(\text{NH}_4)_2\text{SO}_4$, 10-45% soot/HULIS, 30-60% highly fluorescent organics). Overall, the results of our study demonstrate that the RM and the mapping can provide qualitative and quantitative information about the composition of ELPI aerosol samples.

(N. P. Ivleva, U. McKeon, U. Pöschl)



1.4.2 Structural Analysis of Soot and Related Carbonaceous Materials by Raman Microspectroscopy

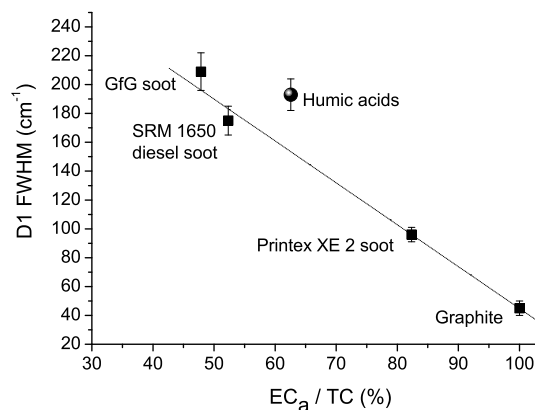
Funding: IWC

Soot particles are hazardous environmental pollutants that account for a major fraction of fine air particulate matter in urban areas. Soot consists mostly of carbon and is composed of agglomerated primary particles with diameters of 10-30 nm that comprise nanocrystalline and amorphous domains. The amorphous domains are disordered mixtures of polycyclic aromatic hydrocarbons and other organic and inorganic components. The chemical composition and structure of primary particles and agglomerates depend on the origin and conditioning of soot.

Raman spectroscopy provides fingerprint spectra, which allow for the distinction of a wide range of chemical substances. The characterisation of graphite-like carbon in diesel soot was first applied by Rosen and Novakov. Since then, several studies reported and discussed the correlation of Raman spectroscopic parameters (such as peak positions, widths, and intensity ratios) with the structure of soot and related carbonaceous materials.

Raman microspectroscopy (which combines the analytical capabilities of Raman spectroscopy with the spatial resolution of an optical microscope) has been applied for the structural characterization of different soot samples (Printex XE2 industrial soot, SRM 1650 diesel soot and GfG spark discharge soot) and related carbonaceous materials (graphite and humic acid). Spectra of investigated samples show pronounced peaks at $\approx 1580\text{ cm}^{-1}$ (G or “Graphite” peak) and $\approx 1350\text{ cm}^{-1}$ (D or “Defect” peak), but the D and G peaks exhibit strongly varying relative intensities and widths. For quantitative spectral analysis we applied the five-band fitting procedure with combination of four Lorentzian-shaped bands (G, D1, D2, D4 at about 1580, 1350, 1620, and 1200 cm^{-1} , respectively) and one Gaussian-shaped band (D3 at about 1500 cm^{-1}). Analysis of spectral parameters revealed a pronounced decrease of D3 band relative intensity (ID_3/IG) with increasing ratio of apparent elemental carbon to total carbon content (EC_a/TC) of the investigated samples, which is consistent with a decrease of the amorphous organic carbon fraction and increase of graphitic structural order from GfG soot (highly disordered) to graphite (highly ordered). Moreover, we found that the D1 band width exhibits a near-linear negative correlation with the EC_a/TC ratio of the soot and graphite samples (see Figure), which is also consistent with an increase of structural order from GfG soot to graphite. The close correlation between width of D1 band and EC_a/TC ratio indicates that Raman spectroscopy may serve as an efficient tool for the characterization of EC_a/TC ratios and the degree of graphitic structural order in soot and related carbonaceous materials.

(*N. P. Ioleva*)



1.5 Microbiology & Microarrays

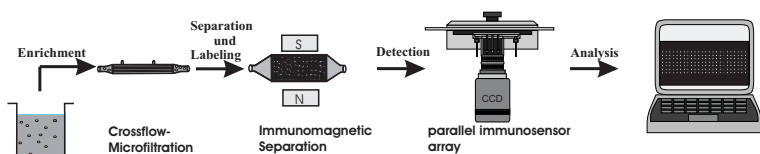
1.5.1 Enrichment of Microorganism in Drinking Water with Crossflow-Filtration

Funding: DFG

The German drinking water regulations of 2001, which came into effect in 2003, require the absence of pathogenic germs in drinking water. Currently, microbiological methods are applied for routine detection. However, these tests are very time consuming (3-7 days) and only indicator organisms like *Escherichia coli*, *Enterococcus* and coliform bacteria are checked regularly. Detection times can be improved from 2h to 2 days depending on sample pre-enrichment required by employing the polymerase chain reaction (PCR) test system as well as enzyme-linked immunosorbent assays (ELISA). For this reason there is a current need for a fast, quasi-continuous and multianalyte test system for the monitoring and quality management of drinking water.

The simultaneous specification and quantification of all relevant pathogenic microorganisms in one single experiment is possible with the microarray technology. The limit of detection of microorganisms for immunosensors lies between $\cdot 10^3$ and $\cdot 10^4$ cfu/mL. German drinking water regulations require the detection of one microorganism in 100 mL drinking water. Therefore it is necessary to make a fast enrichment and purification of 10 L of water up to 100 μ L to obtain this limit of detection.

In this project a quasi-continuous combined system, consisting of crossflow filtration (pre-enrichment), immunomagnetic separation (pre-selection) and parallel affinity sensor array (PASA, quantification), is developed for the detection of all pathogenic and non-pathogenic microorganisms in drinking water.



In contrast to the conventional dead-end filtration, where the feed flow through is perpendicular to the membrane surface, in the cross-flow filtration the feed flows parallel to the membrane surface and part of the retained solutes accumulates. The feed composition inside the module changes as a function of distance in the module, while the feed stream is separated into two streams: permeate and retentate stream.

The choice of the filter unit determines the recovery rate of the microorganisms. This depends on the membrane, the form of the filter module and the transmembrane pressure. For this purpose, a microfluidic device was built up and the transmembrane pressure, feed and Crossflow velocity were adjusted.

At the Institute of Hydrochemistry a parallel affinity sensor array (PASA) for the rapid, automated and simultaneous analysis of a variety of different analytes in fluid samples has been developed performing multianalyte immunoassays on a microarray surface. In this sensor system, chemiluminescence methods are used for detection.

For the quantification of microorganisms in water, an array-based chemiluminescence-sandwich-ELISA has been created. Herein, monoclonal species and subspecies specific antibodies are immobilised on polyethylene glycol (PEG) modified glass surfaces, presenting active groups for covalent coupling. Captured microorganisms are detected by specific secondary antibodies which are labeled with biotin. After the addition of horseradish peroxidase labeled streptavidin and chemiluminescence substrates, the amount of immobilised microorganisms can be quantified at the PASA-system by evaluation of the chemiluminescence signal intensities, detected by a CCD camera.

In order to analyse the used microarray substrates in respect to uniformity, densities

of active surface groups and reproducibility of the glass slide surfaces are validated after each modification step by tagging with biotin derivatives. Measurement of the chemiluminescence signal intensities is again performed at the PASA-system.
(C. Peskoller, A. Wolter, M. Seidel)

1.5.2 Development of a Regenerable Immunosensor Array for the Rapid Parallel Detection of Antibiotics in Milk

Funding: Forschungskreis der Ernährungsindustrie AiF FV 197ZN II

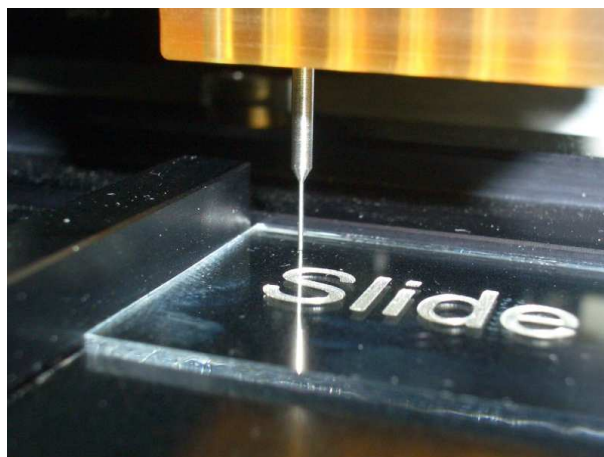
Cooperation: LMU Munich (Prof. Märtlbauer)

Antibiotics are widely used in animal husbandry as growth promoters, for treatment and prophylactics purposes. The presence of antimicrobial residues in food hold the risk of undesirable human health effects. The resulting contamination of milk can result in the occurrence of allergic reactions, bacterial resistance to antibiotics and in the production problems of cultured products (yoghurt and cheese) due to the inhibition of starter cultures. In order to protect the consumer and to maintain food quality, the EU has established residue limits (MRLs) for several antibiotics in bovine milk.

In the past few years, a parallel affinity array (PASA) for the rapid automated analysis of a large number of antibiotics in milk has been developed using multianalyte immunoassays with an indirect competitive ELISA format. Based on this high sensitive biosensor system, a new kind of microarray is developed, where reactive hapten derivatives are immobilised covalently to an activated glass surface via polyethylene glycol (PEG) diamine linkers. In addition to the homobifunctional PEG linkers, heterobifunctional methoxy PEG amines are used for the glass surface coverage. These PEG surfaces are intended to resist unspecific binding of proteins. At the same time, this kind of surface is more regenerable for continuous use than chips based on conventional surface chemistry. To create such a hapten microarray, the glass slide is silanised with 3-glycidyloxypropyl trimethoxysilane after several washing steps. Then the PEG diamine linkers in different molecular weights (2 - 10 kDa) as well as the methoxy PEG amines with shorter chain lengths than the diamine (1 kDa) are attached in varying molar mixing ratios (1:100/ 1:200/ 1:500) to the terminal epoxy groups of the modified glass surface. The PEG coatings are formed in the smelter in a sandwich format. For the direct coupling of the haptens to the free amine groups of the PEG diamine linkers, the haptens must activate first by introduction of NHS ester groups. These haptens are immobilised as tiny spots with a new contact spotting system (Bio-Rad BioOdyssey Calligrapher Miniarrayer) on the activated PEG surfaces. The complete surface treatment and microarray production is optimised and a quality control is implemented.

A new automated chemiluminescence microarray reader is designed in cooperation with gwk Präzisionstechnik. This prototype is constructed as mobile immunosensor array who can measure in parallel 12 different antibiotics in milk.

(K. Kloth, M. Seidel, M. Weller)



2 Publications of Present Members of the IWC

2.1 Journal articles (reviewed)

- T. Baumann and R. Niessner; Micromodel Study on Repartitioning Phenomena of a Strongly Hydrophobic Fluorophore at a Colloid/1-Octanol Interface. *Water Resources Research* 42 (2006) W12S04
- T. Baumann, P. Fruhstorfer, T. Klein and R. Niessner; Colloid Transport at Landfill Sites in Contact with Groundwater. *Water Research* 40 (2006) 2776-2786
- P. Degelmann, S. Egger, H. Jüriling, J. Müller, R. Niessner and D. Knopp; Determination of Sulfonylurea Herbicides in Water and Food Samples Using Sol-Gel Glass Based Immunoaffinity Extraction and LC-UV/DAD or LC-MS/MS. *J. Agric. Food Chem.* 54 (2006) 2003-2011
- C. Haisch, L. Hoffmann and R. Niessner; Design and Characterization of a Highly Directional Photoacoustic Sensor Probe. *Proc. SPIE* 6086 (2006) article no. 60860 E
- D. Knopp; Detection of Trace Metal Ions in Environmental Matrices by Immunological Methods - Review. *Ecol. Chem. Eng.* 13 (2006) 383-397.
- D. Knopp; Immunoassay Development for Environmental Analysis - Trends. *Anal. Bioanal. Chem.* 385 (2006) 425-427.
- D. Matschulat, H. Prestel, F. Haider, R. Niessner and D. Knopp; Immunization with Soot from a Non-combustion Process Provokes Formation of Antibodies against PAHs. *J. Immunological Methods* 310 (2006) 159-170
- A. Messerer, U. Pöschl, R. Niessner and D. Rothe; Soot Particle Deposition Efficiency of Diesel PM-Catalyst Structures - The Influence of Structure Geometry and Transient Temperature Inhomogenities. *SAE Paper Series* 2006-01-3288
- A. Messerer, R. Niessner and U. Pöschl; Comprehensive Kinetic Characterization of the Oxidation and Gasification of Model and Real Diesel Soot by Nitrogen Oxides and Oxygen under Engine Exhaust Conditions. *Carbon* 44 (2006) 307-324
- H. Prestel, R. Niessner and U. Panne; Increasing the Sensitivity of Asymmetrical Flow Field-flow Fractionation (AF4): The Slot Outlet (SO) Technique. *Analytical Chemistry* 78 (2006) 6664-6669
- F. Tsagkogeorgas, M. Ochsenkühn-Petropoulou, R. Niessner and D. Knopp; Encapsulation of Biomolecules for Bioanalytical Purposes - Preparation of Antibody-doped Nanometer-sized Silica Particles by Reverse Micelle and Sol-gel Processing. *Anal. Chim. Acta* 573-74 (2006) 133-137
- R. Niessner, J. Broekaert, J. Einax, H. Emons, W. Engewald, C. Haisch, N. Jakubowski, R. Salzer, W. Schuhmann und M. Weller (2006); Trendbericht Analytische Chemie 2005. *Nachrichten aus Chemie & Technik* 54 (2006) 159-170

2.2 Monographs

- Hiltawsky KM, Haisch C, Mienkina MP, Postema M, Schmitz G. Optoakustik in der medizinischen Bildgebung. In: *Molecular Imaging - Innovationen und Visionen in der medizinischen Bildgebung*; Niederlag W, Lemke HU, Semmler W, Bremer C, Eds. Dresden: Health Academy 2006 (1), 177-192

2.3 Conference Presentations

2.3.1 Oral Presentations

- T. Baumann, H.-L. Paus, J. Teesch, M. Alte & R. Niessner, In-situ Sanierung einer massiven Grundwasserverunreinigung mit Natronlauge, DECHEMA In-Situ Sanierung, 20.-21.11.2006, Frankfurt.
- T. Baumann & R. Niessner, Micromodels: Ein Tool für Prozessstudien zum Transport von Kolloiden, Wasserchemische Gesellschaft, 22.-24.5.2006, Celle.
- T. Baumann, Risikoabschätzung für Grundwasservorkommen bei steigender urbaner und industrieller Nutzung, Fachtagung Wasser 2006, 18.-19.7.2006, Freising.
- C. Haisch, L. Hoffmann, R. Niessner, Design and characterization of a highly directional photoacoustic sensor probe BIOS, Photonics West, 22.01.2006, San Jose, USA.
- N. Ivleva, A. Messerer, U. Pöschl and R. Niessner, Analysis of Changes in the Structure and Reactivity of Soot Undergoing Oxidation and Gasification by Raman Microscopy, 2006 International Aerosol Conference, 10.-15.9.2006, St. Paul, MN, USA
- D. Knopp: Pharmaka im Wasserkreislauf - Neue Targets für immunologische Nachweisverfahren. Analytica Congress 2006, 25.-28. 04. 2006, München.

2.3.2 Poster Presentations

- D. Matschulat, H. Prestel, F. Haider, D. Knopp and R. Niessner; Non-Combustion Soot (NCS) Nanoparticles Generate Highly Affine IgG Class Antibodies Against Polycyclic Aromatic Hydrocarbons Within Vertebrates. 2006 International Aerosol Conference, 10.-15.9.2006, St. Paul, MN, USA.
- C. Kykal, C. Haisch and R. Niessner, Development of a Continuous Aerosol Separation System Based on Photophoretic Particle Properties, 2006 International Aerosol Conference, 10.-15.9.2006, St. Paul, MN, USA

2.3.3 Invited Lectures

- T. Baumann, Visualization of Contaminant Transport in Porous Media, Institut für Bodenkunde und Standortslehre, Universität Hohenheim, 11.12.2006, Hohenheim.
- T. Baumann, Reactive Transport of Colloids on the Microscale, University of Illinois, 14.9.2006, Urbana/Champaign.
- T. Baumann, Reactive Transport of Colloids in Porous Media - The Pore Scale Perspective, EAWAG, 3.7.2006, Zürich.
- C. Haisch, Grundlagen und medizinische Anwendungen der Photoakustischen Bildgebung, Bilder vom Leben: BMBF Biophotonik Symposium 2006, 28.04.2006, München
- C. Haisch, Photoakustik in der Gas- und Aerosolmesstechnik, Deutscher Wetterdienst Lindenberg, 24.10.2006, Lindenberg
- D. Knopp, Pharmaceuticals in the Water Cycle - A New Challenge for Chemical Analysis. Faculty of Chemistry and Chemical Engineering, University Ljubljana, Slovenia, 25.05.2006.

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- D. Knopp, Moderne bioanalytische Methoden: Die Gewinnung und Anwendung von Antikörpern zur Bestimmung von umweltrelevanten chemischen Verbindungen. Department for Marine Bioanalytical Chemistry, Institute for Coastal Research, GKSS Geesthacht Research Center, Geesthacht, 18.08.2006.
- R. Niessner, Selective Analysis by Antibodies and Photons, National University of Singapore, Dept. of Chemistry, 2.3.2006
- R. Niessner, Selective Analysis by Antibodies and Photons, EUROPT(R)ODE VIII, Tübingen, 4.4.2006
- R. Niessner, Laser or Antibodies - Best Friends of Analysts -, Universität Münster, GDCh-Vortrag, 10.4.2006
- R. Niessner, Immunochemical Techniques for Monitoring Contaminant Traces, 34th Intern. Symp. on Environmental Analytical Chemistry, Hamburg, 6.6.2006
- R. Niessner, Selective Analysis by Antibodies and Photons, Intern. Symp. on Luminescence Spectrometry and Detection Techniques in Biomedical, Environmental and Food Analysis, Lugo (Spain), 21.7.2006
- R. Niessner, The History of Aerosol Photoemission, 3rd Symp. on the History of Aerosol Science, St. Paul (USA), 8.9.2006
- R. Niessner, Laserlight or Antibodies: The Best Friends of Analysts, Indiana University, Chemistry, Department, Bloomington (USA), 19.9.2006
- R. Niessner, Soot: For Analysts a Hard Nano-nut to Crack?, Workshop on Atmospheric Soot: Environmental Fate and Impact 2006, Arcachon (France), 19.10.2006
- R. Niessner, Soot, For Analysts a Hard Nano-nut to Crack?, Universität Duisburg-Essen, GDCh-Vortrag, 29.11.2006
- R. Niessner, Trends in Immunoanalytical Techniques for Fast Screening, La Rete dell'Alta Tecnologia dell' Emilia-Romagna, Ferrara (Italy), 5.12.2006
- M. Seidel: Assay Principles in Bioanalysis. CareMan Summer School "Fluorescence and Biomolecules", 24.-27.9.2006, Tübingen.

2.4 Hydrogeological Consulting

Mineralisation control analyses Bad Abbach, Bayreuth, Bad Birnbach, Bad Endorf, Bad Füssing, Bad Griesbach, Bad Gögging, Bad Rodach, Sybillenbad, Bad Staffelstein, Straubing, Bad Tölz, Utting, Bad Wiessee, Bad Wimpfen

Hydrogeological and hydrochemical expertises (mineral water, spa water) Bad Tölz, Bad Gögging, Bad Brückenau, Hölle, Sibyllenbad, Hohenberg/Eger, Füssen, Lipik (Kroatien)

Deep Hydrogeothermal Energy Exploration Erding, München-Riem, Pullach, Bad Wörishofen

2.5 Bachelor Theses

T. H. Nguyen: Bestimmung des Kreuzreaktivitätsprofils isolierter IgG-Subfraktionen eines Diclofenac-Antiserums

2.6 MSc and Diploma Theses

- E. Bucur-Eriksson: Development of a Measurement Device for Analysis of the Caseous Compounds of the Mikrobiological Hydrogen Fermentation
- M. Damyanov: Untersuchung der hydraulischen und hydrochemischen Verhältnisse im Höllental
- R. Hentschel: Hydrochemische Verhältnisse im Malmaquifer in Oberbayern
- L. Hoffmann (LMU): Aufbau und Charakterisierung eines photoakustischen Sensors zur Tiefenuntersuchung optischer Inhomogenitäten
- S. Jähme (LMU): Streulichtmessungen zur Detektion von Bakterien in Grundwasser
- Z. Li (GIST): Evaluation of New Protein Labels for Quantitative Proteomics Based on Mass Spectroscopy
- C. Peskoller: Herstellung und Charakterisierung von Affinitätsmonolithen für die Anwendung der Chromatographie

2.7 PhD Theses

- Dipl.-Chem. D. Rothe: Physikalische und chemische Charakterisierung der Rußpartikelemission von Nfz-Motoren und Methoden zur Emissionsminderung
- Leb.-Chem. M. Kiening: Immunanalytische Methoden zur Detektion von Erdnuß- und Haselnuß-Spuren in Lebensmitteln
- Dipl.-Chem. T. Fehrenbach: Analyse von Aminosäuren, Proteinen und Nitroderivaten in atmosphärischen Aerosolen und in Straßenstaub

2.8 Habilitation Theses

- T. Baumann, Aquatic Colloids – Relevance for Transport Processes in Groundwater, Habilitation Thesis, TU München
- U. Pöschl, Carbonaceous Aerosol Composition, Reactivity, and Water Interactions, Habilitation Thesis, TU München

3 Teaching, Colloquia, and Other Activities

3.1 Classes

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

- Analytical Chemistry - Physical and Chemical Separation Methods (Analytische Chemie - Physikalisch-chemische Trennmethoden); Niessner
- 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

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- Biochemical and Molecular Biological Procedures for Environmental Analysis II - Enzymatic Methods, DNA Probes (Biochemische und molekularbiologische Verfahren in der Umweltanalytik II - enzymatische Verfahren, DNA-Sonden); Knopp
 - Hydrogeological, Hydrochemical and Environmental Analytics Seminar (Hydrogeologisches, Hydrochemisches und Umweltanalytisches Seminar); Niessner, Baumann
 - Graduate Course in Analytical Chemistry: Organic Trace Analysis Lecture (Vertiefungsfach Analytische Chemie: Vorlesung Organische Spurenanalytik); Niessner
 - Graduate Course in Analytical Chemistry: Organic Trace Analysis Lab (Vertiefungsfach Analytische Chemie: Praktikum Organische Spurenanalytik); Niessner, Seidel
 - Trace Analysis Techniques (Spurenanalytische Techniken); Niessner
 - Water Chemistry Lab II (Wasserchemisches Praktikum II); Niessner, Haisch, Knopp, Seidel

3.1.2 Chemical Engineering (Diplom)

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

3.1.3 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
- Introduction to HYdrogeology (Ringvorlesung Geowissenschaften); Baumann
- 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

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- Numerical Methods Lab (Hydrogeologische Modellierung II); Baumann
 - Hydrogeological Field Lab (Hydrogeologische Feldmethoden); Baumann, Haisch
 - Hydrogeological Mapping (Hydrogeologische Kartierung); Baumann, Haisch
 - Hydrogeological, Hydrochemical and Environmental Analytics 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

3.1.4 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

3.2 Institute Colloquia

Dr. rer. nat. Andrea Büttner, Deutsche Forschungsanstalt für Lebensmittelchemie an der TU München: Retronasal Aroma Perception Considering Physiological Aspects - Application of MRI, Videofluoroscopy and PTR-Mass Spectrometry (18.1.2006)

Dr. Thomas Schäfer, Bundeskriminalamt Wiesbaden: Einsatz der Analytischen Chemie in der Kriminaltechnik (25.1.2006)

Prof. Dr. med. Peter Lippa, Lehrstuhl für Klinische Chemie, TU München: Kinetische Analyse der biospezifischen Interaktion zwischen Steroidhormonen und Steroidbindenden Proteinen mittels SPR-Biosensorik (14.2.2006)

Dr. Brischwein, Heinz Nixdorf-Lehrstuhl für Medizinische Elektronik, TU München: Cell-based Assays: Mikrosensorarray-basiertes Screening an lebenden Zellen und Geweben (16.2.2006)

Dr. Frances S. Ligler, Naval Research Laboratory, Center for Bio/Molecular Science & Engineering, Washington: Array Biosensor (6.4.2006)

Prof. Dr. Thorsten Benter, FB C - Physikalische Chemie Bergische Universität Wuppertal: Real-time Analysis of Gas Constituents by REMPI-MS (8.5.2006)

Prof. Dr. Roland Zengerle, Institut für Mikrosystemtechnik, Universität Freiburg: Microfluidics: From Ultra-Highly-Parallel Dispensing to Automation of Miniaturized Assays (12.5.2006)

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- Dr. Martin Elsner, GSF - Institute of Ground Water Ecology, Neuherberg: From Degradation Pathways to Reaction Mechanisms: Use of Compound Specific Isotope Analysis in Environmental Chemistry (12.6.2006)
- Prof. Dr. Edgar A. Arriaga, Max Planck Institut für Biochemie, Martinsried: Measuring the Properties of Individual Biological Particles by Capillary Electrophoresis (14.6.2006)
- Dr. Amr Abdel-Fattah, Chemistry Division, Los Alamos National Laboratory, USA: Studies on Colloid Deposition onto a Solid Surface using the Automated Video Microscopic Imaging and Data Acquisition System (AVMIDAS) (20.6.2006)
- Dr. Daniel P. Funeriu, Dept. Chemie, TU München: Enzyme Chip Development for Effector Screening (27.6.2006)
- Prof. Dr. Ulrich Tallarek, Institut für Verfahrenstechnik, Otto-von-Guericke-Universität Magdeburg: Electrokinetic Phenomena in Miniaturized Separation Systems (9.10.2006)
- Dr. Goestar Klingelhofer, Institut für Anorganische und Analytische Chemie, Johann-Gutenberg-Universität Mainz: Water on Mars - Results from the Mars-Exploration-Rover Mössbauer Spectrometers MIMOS II (24.10.2006)
- Dr. Herbert Oberacher, Institut für Gerichtliche Medizin, Universität Innsbruck: High Performance Mass Spectrometry of Nucleic Acids Possibilities and Limitations in Genome Research (30.10.2006)
- Dr. Andreas Volkmer, 3. Institut für Physik, Universität Stuttgart: CARS Microscopy - Insight into the Unseen of Living Cells (15.11.2006)
- Dr. Conrad Coester, Dept. for Pharmacy, Pharmaceutical Technology and Biopharmaceutics, LMU München: New Biocompatible Nanoparticles as Drug Delivery Systems for Nucleic Acids, Peptides and Proteins (13.12.2006)
- Prof. Dr. Michael Köhler, Institut für Physik, Technische Universität Ilmenau: Micro Flow-through Devices for Chemical Synthesis and Biological Screening (20.12.2006)

3.3 External Tasks and Memberships

Prof. Dr. Reinhard Niessner

Bayer. Fachausschuß für Kurorte, Erholungsorte und Heilbrunnen	Member
DECHEMA Commission "Chemische Grundlagen und Anwendungen der Sensortechnik"	Member
DFG-Senatskommission für Wasserforschung	Member
Heinrich-Emanuel-Merck-Award Committee	Jury Head
Smoluchowski-Aerosol-Award Committee	Jury Head
Bayer. Institut für Abfallforschung, Augsburg	Advisory Board Member
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
Analyst	Advisory Board Member

PD Dr. Thomas Baumann

Bayer. Fachausschuß für Kurorte, Erholungsorte und Heilbrunnen	Member
VBGW AK Grundwasserschutz	Member
Taskforce "pHOENIX" in the International Waste Working Group	Member
"AK Kolloide" in the Hydrochemical Society	Member
DIN NA 119-01-02-05 UA Leaching	Member

Prof. Dr. Dietmar Knopp

KRdL-3/7/04, "Luftgetragene Mikroorganismen und Viren", im VDI/DIN	Member
Ecotoxicology and Environmental Safety	Editorial Board Member
Chromatographia	Editorial Board Member

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 Laser

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

4.2.2 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 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

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- 3 Intensified CCD cameras
 - 1 Wavemeter

4.2.3 Chromatography

- 7 GCs with FID, NPD, ECD, TEA and AED
- 1 GC/MS, block-injection and autosampler
- 1 High-resolution GC/MS, VG Autospec
- 1 LC-Orthogonal-ESI-TOF-MS, Micromass
- 1 Lyophilizer
- 1 Asymmetrical Field-flow-fractionation system
- 1 SFE-System with modifier, Suprex
- 2 Concentrators for dynamic headspace analysis
- 1 High-speed counter-current-distribution chromatographic system
- 3 HPLC, UV/VIS array detector, programmable fluorescence detector
- 2 HPLC
- 1 Capillary electrophoresis system
- 1 Ion chromatograph, Dionex 4500 i
- 1 Ion chromatograph, Dionex BioLC (Photodiode Array Detector, Electrochemical Detector)
- 1 AMD system for HPDC with UV, VIS and fluorescence scanner
- 1 LC system, ECONO
- 1 Preparative HPLC

4.2.4 Dioxin Laboratory

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

4.2.5 Bioanalytics

- 2 Fluorescence reader systems, time-resolving
- 3 Photometric reader systems
- 1 Chip spotter system, GeSIM
- 1 384-channel washer, Biotek

4.2.6 Element Analytics

- 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

4.2.7 SEM/Microscopy/Colloid Sizer

- 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)
- 1 Zetaphoremeter, SEPHY

4.2.8 Sum Parameters

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

4.2.9 Aerosol Research

- 1 Aerosol chamber (1 m³)
- 1 Aerosol flow tube (10 L)
- 1 Ozone analyzer (UV absorption)
- 1 NO/NO₂ analyser (Chemiluminescence)
- 2 Aerodynamic particle sizers (0.5-25 μm)
- 1 Berner impactor (9 stages, 50 nm - 16 μm)
- 1 Electrical low-pressure impactor (12 stages, 30 nm - 10 μm)
- 2 Low-Volume filter samplers (PM 10, PM2.5)
- 1 High-Volume filter sampler (PM 2.5)
- 2 Differential mobility particle sizer systems (10-1000 nm)
- 2 Diffusion batteries (5-300 nm)
- 5 Condensation nucleus counters
- 3 Electrostatic classifiers (10-1000 nm)
- 2 Spark-discharge soot aerosol generators (polydisperse ultrafine carbon aerosol)
- 1 Berglund-Liu aerosol generator (monodisperse aerosols, 0.8-50 μm)
- 1 Floating bed aerosol generator (powder dispersion)
- 1 Rotating brush aerosol generator (powder dispersion)

4.2.10 Microbiology

- 1 Clean bench (Herasafe KS, Kendro)
- 1 Ultra Low Freezer (B35-85, Thermo Electron Cooperation)
- 1 Refrigerated Incubator Shaker (C24 KC, New Brunswick Scientific)
- 1 Microbiological Incubator (BD 53, Binder)
- 1 Autoclave (Century 2100, Prestige Medical)
- 1 Lyophilizer (Alpha 1-4 LSC, Christ)
- 1 Washer Disinfectant (DS 500 Lab, International Steel CO.SPA)
- 1 Ultrapure Water System (Direct-Q 3 UV, Millipore)
- 1 Refrigerated Centrifuge (Universal 320R, Hettich)
- 1 Microarrayer (BioOdyssey Calligrapher Miniarrayer, Bio-Rad)

5 Staff 2006

Univ.-Prof. Dr. Reinhard Nießner
PD Dr. Thomas Baumann
Dr. Christoph Haisch
Dr. Andreas Held (until 6/06)
Dr. Natalia Ivleva
Prof. Dr. Dietmar Knopp
PD Dr. Ulrich Pöschl (until 3/06)
Dr. Harald Prestel (until 3/06)
Dr. Michael Seidel
PD Dr. Michael Weller (until 8/06)

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

Hatice Hazir
Mira Kolar

PhD Students

Dipl.-Chem. Christian Cervino
Dipl.-Chem. Susanne Fabel (until 2/06)
Dipl.-Chem. Tobias Fehrenbach (until 2/06)
Dipl.-Ing.FH Clemens Helmbrecht
Dipl.-Chem. Katrin Kloth
Dipl.-Chem. Markus Knauer (from 10/06)
Dipl.-Met. Carsten Kykal
Dipl.-Chem. Caroline Peskoller
Dipl.-Chem. Philipp Stolper
Dipl.-Chem. Zhe Sun
MSc Laura Toops
Dipl.-Chem. Anne Wolter
Dipl.-Phys. Karin Zell

External PhD Students

Apotheker Alexander Buhl (TUM, Klin. r. d. Isar)
Dipl.-Biol. Melanie Maier (GSF)
Dipl.-Phys. Peter Menzenbach (INNOLAS, Krailling)
Dipl.-Biol. Roman Radykewicz (GSF)
Staatl.gepr.Leb.-Chem. Michael Rampfl (IBP Holzkirchen)
Dipl.-Chem. Tobias Roßteuscher (z.Zt. Prof. Kitamori, Tokyo University)

Diploma Students/MSc Students

Marian Damyanov (4/06 until 7/06)
Rolf Hentschel (2/06 until 9/06)
Leonard Hoffmann (until 1/06)
Sebastian Jähme (until 6/06)

External Diploma Students

Zhen Li (LaRoche) (from 9/05)

Bachelor Students

Thanh Huyen Ngyen (Chemistry)

Guests and Research Fellows

Dr. Minli Yang, University Peking
Christoph Leidig, LMU

Student Assistants

Okroy Andrea (from 10/06)
Wolter Wolfgang (from 10/06)
Kreissig Johanna (from 10/06)