TECHNISCHE
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MÜNCHEN

Institute of Hydrochemistry

Chair for Hydrogeology, Hydrochemistry and Environmental Analytical Chemistry

Annual Report

2004

Head of the Institute and Group Leaders 2004

T. Schmid, D. Knopp, C. Haisch, U. Pöschl, T. Baumann, M. Weller, R. Nießner

Institute of Hydrochemistry
Chair for Hydrogeology, Hydrochemistry and Environmental Analytical Chemistry
Technische Universität München
Marchioninistr. 17

D–81377 München

Editor: Dr. Thomas Baumann

Editorial

Dear coworkers, friends and colleagues,

this year was certainly a ambitious one. We were facing multiple challenges: changes of our education system (diploma course into bachelor/master system), significant cuts in research funding, and continuously decreasing numbers of PhD students.

With the bachelor programme in geosciences, together with LMU, the student numbers doubled. Positively seen is here the extended teaching in analytical and organic chemistry. I'm sure we will benefit from this within the next years. Teaching in Singapore (Industrial Chemistry) became routine, right now two master students from there are working on their master thesis at our institute. Quite similar happened with the Chemical Engineering programme at TUM, where the aerosol group is mainly involved. Several diploma theses are conducted in this field. The next year will see the change to BS/MS system in Chemistry and Chemical Engineering, which will again stress our capacity. The new policy of directing the TUM resources (e.g. yearly funding for consumables) in favor of chairs with a highly education oriented profile will certainly not strengthen the leading scientific position of TUM chemistry worldwide. Analysis of the recently granted professorships at TUM also exhibits a trend of decreasing funding for establishing new colleagues. Meawhile, the start up grants have been cut to roughly 50 % compared to 1990. In this sense a dramatic change toward the American system is observed. It can be extrapolated that within 20 years a chemistry faculty (if still existing at TUM) consists of about 25 working groups, with small time-limited resources. Whether this will be attractive and stimulating for our best young scientists and will motivate them to start an academic career, is highly questionable.

This year the total number of coworkers declined from 51 at the beginning of 2004 to 43 at the end of this year. This is due to the number of Post Docs and PhD students at the institute: dropping from 30 in January to 22 in December. Over the year we hosted about 6 - 8 diploma (master) students, a number which seems to be stable. Unfortunately only a very few of them are willing to start a PhD thesis. This was observed more and more during the last year: "volatility" seems to be trendy. Nevertheless, 5 PhD works were successfully finished this year, and the freshly appointed chemists, pharmacist, physicist and food chemist are all under contract.

Very positive in this relation was the appointment of my long lasting coworker Dr. Ulrich Panne as the new Head of the Chemical Division of the Federal Institute for Material Testing (BAM) in Berlin, combined with the Chair for Analytical Chemistry at Humboldt University. A real breakthrough in our discipline for the first time. Others competing for a professorship this year were nearly succeeding: next year the time for applying is coming (right now 3 analytical chairs are open . . .). Due to a contract with TUM we could replace Dr. Panne's permanent position by Dr. Haisch. Hence, the long lasting laser spectroscopy competence is continuing.

Research funding is drastically cut down. At present we have the unpleasant situation that even at low funding not all open PhD positions are occupied. Here we have clearly to focus our efforts. Without PhD students we will not have new impact and ideas. A clear indicator for research power can be seen in the number of publications released. About 20 this year reflects the decreasing number of scientists present at the institute, folded with increasing teaching loads. Most of these publications are published in high impact number journals, a policy which is now fully adapted by the institute.

A highlight was the world-wide launching of the photoacoustic diesel exhaust aerosol sensor by AVL Graz, Austria. Here, after about 12 years development, an idea became successfully converted into an widely accepted product. It is currently the only means to monitor the exhaust limitations continuously. A very satisfying project, indeed!

The other strategic project is the protein chip. Faced to a heavy world-wide competition in this field a complete chip technology (production of the protein chip and read-out) is demonstrated. Here we hope to see a breakthrough within the next 3 years. In the field of antibody production, the key to sensor or chip technologies for fast screening for contaminants, especially the microcystin antibodies are requested. Our long lasting commitment to go the “antibody way”, obviously was right.

What is planned for the next year? A brief look into our technical hall tells you, that microbiology has reached analytical chemistry. The characterisation of biological analytes (viruses, microorganisms, high-molecular weight proteins released from “living” organisms) are the demands of tomorrow. Mid of February 2005 the building of a microbiology lab will be finished. We will use it as a nucleus for extending our capabilities in the area mentioned above.

Finally, I like to express my sincere thanks to all who contributed to our success experienced so far. Especially the permanent staff is thanked for trusting and helping me, right when the pressure on my shoulders became hard and unresistably this year . . .

Reinhard Nießner
Head of the Institute

1 Research

1.1 Hydrogeology and Hydrochemistry

1.1.1 Development and Protection of Ground Water and Mineral Water

Funding: Private Enterprises

The concurrent use of groundwater ressources, e.g., the use of thermal water for geothermal energy production as well as for medicinal baths, or the exploration of mineral water aquifers with several wells, requires sound understanding of the hydrodynamic and hydrochemical processes in aquifer systems.

The implementation of aquifer and well management systems have been proven a suitable tool to assess the interactions between different groundwater or mineral water wells. Although the gathering of data is time and labour intensive, such a management system is fundamental for sustainable groundwater use and for risk assessment tools. Detailed knowledge of the well characteristics in a multi-well environment is also indispensable for emergency plans to ensure mineral water production if wells fail or during maintenance.

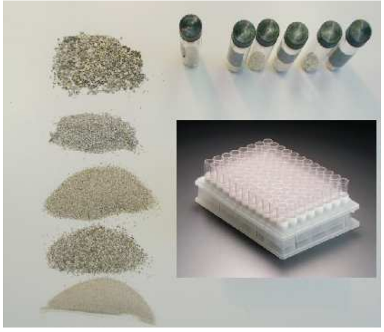
Research is focused on tailored management and risk assessment applications to ensure sustainable development of groundwater ressources.

Groundwater and mineral water exploration was again bringing together the field experience of classical hydrogeologists and the modelling skills of applied hydrogeology. Groundwater protection against anthropogenic influence has to be taken into account at an early stage to ensure the purity of the mineral water. This leads to remote exploration or usage of deep groundwater aquifers.
(*T. Baumann*)

1.1.2 Development of a High-Throughput Test Design for the Determination of Sorption Parameters

Funding: IWC

Sustainable development of pesticides, pharmaceuticals, and other industrial chemicals implies the reduction of long-term environmental risks. Therefore the environmental fate of newly developed substances has to undergo a strict assessment and prediction.



Natural environments are characterized by their spatial chemical and physical heterogeneity. Therefore it seems to be impossible to predict, e.g., the transport of an antibiotic under all possible circumstances. However, natural heterogeneity can be seen as problem of combinatorics with a limited number of unique components and settings.

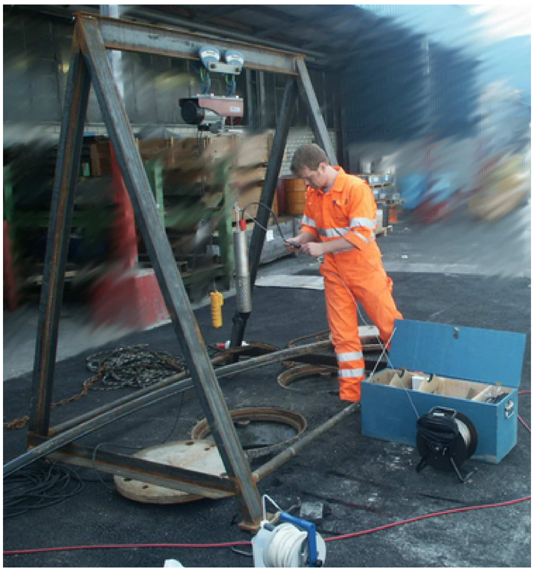
With the development of a high-throughput sorption test we now are able to measure the matrix interactions of chemical substances in parallel. Therefore, one major drawback of the combinatorical approach, the vast number of initial samples, can be overcomed.

Ongoing research is focused on the scalability of this approach. The accessibility of the matrix components has already been identified as one target. Another issue is the characterisation of typical regional matrix settings and their transformation onto the sorption test.
(*O. Fenton, T. Baumann*)

1.1.3 Assessment and Remediation of a pH-Anomaly in Groundwater

Funding: Private Enterprises

At an industrial site a spill of caustic soda caused high pH values in the upper groundwater aquifer. The main water supply of the company was at risk due to a transition of the carbonate equilibrium causing the development of carbonates scalings at the production wells. Early remediation activities were based on pump-and-treat techniques. However, the operation times of the wells and pumps were extremely short (hours to days).



Site assessment with a multiparameter probe revealed a stratified contamination. While the upper part of the phreatic aquifer showed natural pH values between 7.5 and 7.8, the pH values rised to 10 and 11 at the bottom of the upper aquifer. The transition zone between the uncontaminated groundwater and the contamination was usually less than 50 cm thick. The aquifer bottom was found to have a pronounced morphology with highs and lows. After the site assessment we came to the conclusion, that the caustic soda propagated through the unsaturated and the saturated zone to the bottom of the aquifer driven by the higher density. At the bottom of the aquifer pools of caustic soda were formed in morphological lows. At this state, without remediation measures, the release of the caustic soda was diffusion controlled.

After the initial site assessment the unconditional pump-and-treat technique was redesigned. The new groundwater wells had their filter screen in the contaminated lower part of the aquifer. With an increased number of wells the drawdown at the individual well was reduced, thus reducing the mixing of contaminated and uncontaminated groundwater. Finally carbon dioxide was injected close to the remediation wells to prevent carbonate precipitation.

As a result of these measures, the operation times of pumps and remediation wells was increased dramatically. As a side effect of the amount of contaminated water was reduced, since mixing in the aquifer and in the well was reduced significantly. The risk of a propagation of the contamination to the main water supply was effectively reduced.

The field work was backed up by lab and pilot scale experiments to study the transport of reactive gases in a porous system. Based on the kinetics of carbonate dissolution and precipitation a hydrogeochemical model was calibrated using the surface-to-volume ratio of the precipitates as a fitting variable. The results were in agreement with measured colloid diameters.
(*M. Alte*)

1.1.4 Characterization of Hydrocolloids Using Slot Outlet-Asymmetrical Flow Field-flow Fractionation (SO-AF4) and ICP-MS

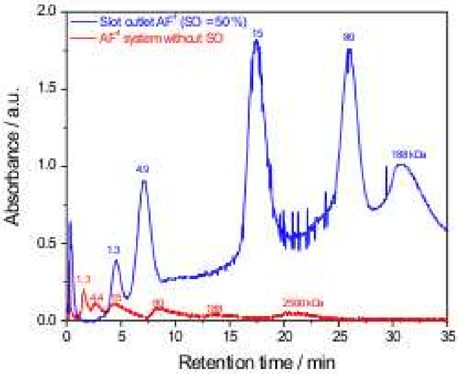
Funding: DFG Pa-716/4-2
Cooperation: Institute of Water Quality Control and Waste Management, TUM (Prof. Wilderer)

The goal of this project is the characterization of artificial and natural hydrocolloids, especially in municipal and industrial waste water treatment plants, and the investigation of their interactions with biofilms in laboratory reactors and technical plants.

Field-flow fractionation (FFF) permits a fast size-selective separation of colloids under very careful conditions. For multi-element analysis, especially the size distributions of heavy metals in natural hydrocolloids, the AF4 system was combined with online inductively-coupled plasma mass spectrometry (ICP-MS). The size distribution is determined by AF4 with UV absorbance and fluorescence detection and compared with the size information obtained by ICP-MS detection.

In all FFF sub-techniques dilution in the separation channels (in asymmetrical flow-FFF (AF4) up to 1000fold) causes signal decrease. To minimize this problem, a new technology, the so-called slot outlet technique (SO) was established. This technique is based on that during fractionation the colloids are located in the bottom 10μm of the separation channel. So removal of sample-free carrier sub-stream increases the colloid concentration of the other substream. This is achieved by splitting the carrier at the end of the channel using a slot outlet, and enables a signal increase up to 24fold (see figure). Additionally better resolution, especially in the range between 1 kDa and 100 kDa, could be achieved by using a new focusing technique, and other cross flow gradients.

The new SO-AF4 system was applied to characterize natural hydrocolloids from different sewage plants. Other applications were the characterization of heavy metal phosphate tracer colloids, drug-coated magnetite particles, and polymers. The results have shown that the SO technique improves the AF4 sensitivity and resolution with and without ICP-MS online coupling.



Additionally the synthesis of monodisperse thulium(III)phosphate colloids by slow increase of pH in solutions containing soluble rare earth metal salts and phosphoric acid, which has been developed last year, has been optimized. First experiments with sewage plant samples and in river water have been carried out to estimate the use of those particles as tracer colloids. Investigations with different tracer colloids at three biofilm reactors were made to receive informations about interactions of tracer colloids with biofilms.

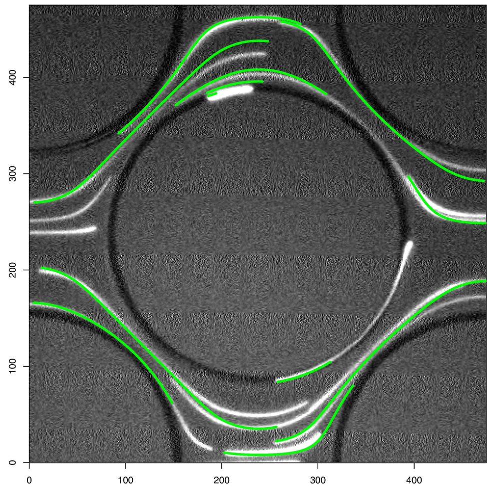
(*H. Prestel*)

1.1.5 Single Particle Analysis to Assess Colloidal Transport

Funding: DFG Ba 1592/3-1

Regardless of the scale of colloid transport experiments, from the field scale with flow lengths of more than 100 m down to pore scale with single particle analysis, the most frequently asked question is about upscaling/downscaling.

While heterogeneity of different origin is intrinsically covered in large scale experiments, a completely different experimental setup has to be applied for single particle experiments rising problems not only with data aquisition, but also with numerical modelling.



Current research is therefore driven by the idea of providing an experimental link between the different scales. In meantime we arrived at the micro scale, where particle-matrix interactions are almost directly accessible.

Colloidal transport in the saturated and unsaturated zone of porous aquifers is known to affect the transport of contaminants. It is therefore of great interest to predict colloidal transport phenomena.

Micromodels, i.e. porous structures etched in silicon wafers, provide the possibility for a single particle analysis of colloid-matrix interactions under various conditions. Thus, the processes taking place at the interfaces seem to be accessible.

Work already performed includes transport studies for colloids in physically homogeneous and heterogeneous pore structures. Work planned is focussing on chemically heterogeneous pore structures, multi-phase systems and colloid-biofilm interactions.

First results are in good agreement with the theoretical framework of colloidal transport. The results also indicate, that some of the problems experienced when applying the theory to bulk scale experiments like column or field test arise from an inapproproiate description of the processes at the pore scale.
(*J. Arágon-Gómez*)

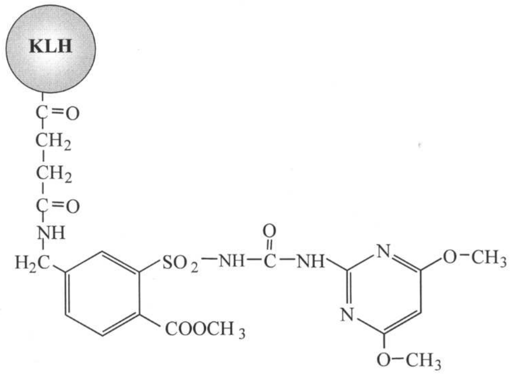
1.2 Bioanalytics I

1.2.1 Determination of Sulfonylurea Herbicides Using Combined Immunoaffinity Extraction-Liquid Chromatography-MS

Funding: DFG Kn 348/8-1 (with support from Dr. J. Wenger, Syngenta, Basel)
Cooperation: Fraunhofer Institute of Molecular Biology and Applied Ecology, Schmallenberg (Dr. J. Müller)

Sulfonylureas (SUs) are a class of herbicides, that are popularly used for a variety of crops because of their high herbicidal activity and low toxicity to mammals. If used in accordance with label directions, these herbicides do not constitute an important environmental and mammalian hazard. However, if improperly applied, or after accidental events, higher amounts of herbicides can reach both surface water and groundwater. Because of the low use range and their chemical characteristics such as thermal instability, monitoring of these herbicides in environmental samples needs techniques for sample enrichment and purification prior to chromatographic analysis.

One of the aims of the present project was to prepare antibodies of broad specificity for SUs which can be used to establish a class-specific ELISA for rapid and cost-effective sample monitoring and, at a later stage, for selective analyte enrichment.



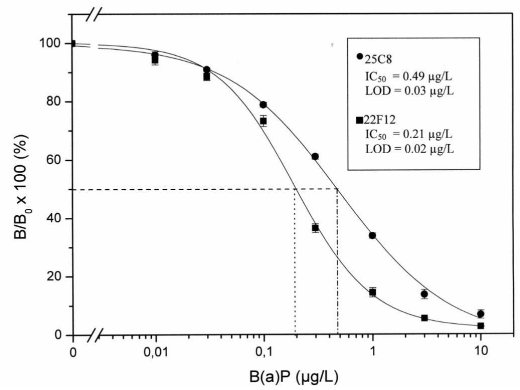
In this project, antibodies could be prepared against sulfonylurea herbicides using a complete molecule or only different structural parts as haptens. Antiserum with the broadest specificity was obtained with a mesosulfuronbenzylamine derivative which was coupled via a succinic acid spacer to KLH. A heterologous enzyme tracer which did not contain the succinic acid bridge was prepared using activated horseradish peroxidase. Using the optimized direct ELISA from 30 SUs, 8 compounds showed a molar cross-reactivity higher than 100% (this value was set for the hapten) and 11 compounds CRs between 10% and 100%. The ELISA can detect 16 SUs at a concentration of 0.1 μg/L or lower. Correlation analysis (ELISA vs. HPLC) of spiked surface and tap water samples revealed good agreement between both methods ($r^2 > 0.948$, n=21). Using ELISA, no sample pretreatment other than filtration was necessary.
(*P. Degelmann*)

1.2.2 Preparation of Monoclonal Antibodies with High Selectivity for the Polycyclic Aromatic Hydrocarbon Benzo[a]pyrene

Funding: BMBF 02WU0290

Because of their carcinogenicity and ubiquitousness in the environment polycyclic aromatic hydrocarbons (PAHs) have caused increasing attention in recent years. In the Council Directive 98/83/EC concerning the quality of water intended for human consumption (Drinking water directive) a limit value of 10 ng/L (10 ppt) was set for benzo(a)pyrene (B(a)P) which is the lowest of all limit values set for individual chemical parameters in this directive. This limit value and all the rest of them have to be redeemed at the faucet i.e. at the customer and, therefore, possible effects of the distribution network on the water quality have to be considered. In many countries, tarred water pipes are still in use, although they were installed decades ago. In Germany e.g. the percentage is estimated to be about 5% of the actual stock. The coal tar layer protects pipes from corrosion but, as a disadvantage, may be a source of contamination of the flowing through water with PAH.

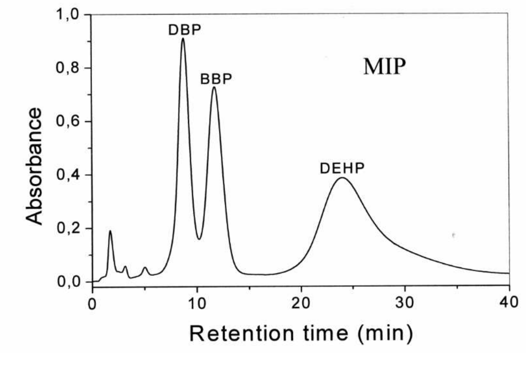
Because of the low limit value, sensitive and reliable analytical methods are needed to evaluate the presence of B(a)P in tap water. Generally, gas chromatography (GC) and high-performance liquid chromatography (HPLC) are used which need pre-concentration of analyte and are relatively time-consuming and difficult to perform on-site. In contrast, immunoassays are typically highly sensitive and comfortable to implement provided that an appropriate antibody is available. Only a few papers focussed on the generation of antibodies rather specific for individual PAH compounds and B(a)P was the center of interest. Recently, we reported on the generation of a very broad-specific monoclonal antibody for PAH and its application for the determination of these chemicals in aerosol extracts which contain a variety of different PAH. As the hapten, for the first time a B(a)P derivatized with a C4-spacer in 1/3-position of the B(a)P was used. However, beside of the broad recognition of different PAH also the sensitivity of the corresponding ELISA for B(a)P did not comply the new limit value set for this analyte in tap water. Therefore, it was the aim of this study to generate a new monoclonal antibody with distinct higher specificity for the target analyte compared to other relevant PAH and high affinity to allow most sensitive detection of B(a)P. This was achieved by immunization with novel conjugates prepared with new benzo[a]pyrene derivatives. Calibration graphs of the best two monoclonal antibodies generated in this project are depicted in the figure.
(*D. Matschulat, A. Deng*)



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

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

The subproject focusses on the synthesis of molecularly imprinted polymers (MIPs), which can be considered as artificial antibodies, for polycyclic aromatic hydrocarbons (PAH) and phthalate esters (PE). Benzo[a]pyrene (B[a]P) is one of the best known carcinogenic PAH. It is generally formed by incomplete combustion and pyrolysis of organic materials. It also has been detected in tobacco smoke, sediment, soils, water, air, marine organisms and even food stuffs. Diesters of phthalic acid, commonly known as phthalate esters (PE) or phthalates, are produced worldwide in large quantities and used e.g. as plasticizers, i.e. to give the synthetic materials its desired flexibility. Di(2-ethylhexyl)phthalate (DEHP) is of most importance. Nonoccupational exposure can occur with the use of a vast range of consumables such as personal-care products, paints, industrial plastics, certain medical devices and pharmaceuticals.



Six kinds of MIPs in the form of bulk polymers or microspheres were synthesized with B[a]P as template and using different functional and cross-linking monomers. 4-Vinylpyridine and divinylbenzene together with dichloromethane as porogen revealed as the best combination. The prepared MIP could be applied to real samples such as surface water and food samples (instant coffee) to extract the target analyte from these samples.

From the MIPs which were prepared with different phthalates the DEHP-MIP was by far the best one (capacity factor of 15.9 and imprinting factor of 8.0). As shown in the figure, if it was used as packing material for HPLC columns, a mixture of three phthalates was almost baseline separated, with highest retention (affinity) for DEHP.
(*J.-P. Lai, M. Yang*)

1.2.4 Preparation and Characterization of Arsenic Conjugates

Funding: IWC

Arsenic is the twentieth most abundant element in the earth's crust. The most toxic form of arsenic is inorganic arsenite (As(III)) which is approximately ten times as toxic as inorganic arsenate (As(V)) and one hundred times as toxic as the typical organic forms of arsenic. In water, depending on the redox condition, the most prevalent species of arsenic are anionic or neutral inorganics. Usually, the concentrations in the environment and biological systems are very low (low ppb-range). However, millions of people in Southest Asia are still being exposed to high levels in their drinking water. Therefore, analytical methods must develop to monitor the different chemical forms.

Speciation is an analytical challenge because of several reasons. First, species concentrations are generally low. Second, species may change during sample treatment and, third, sample matrix may interfere with the analytical method. Contamination must be prevented, and loss of trace analytes must be minimized. In ideal procedure might therefore guarantee the identification of species and the preservation of orignal state of species. Of the numerous methods reported, liquid chromatography-inductively coupled plasma mass spectrometry (LC-ICP-MS) with high sensitivity and accuracy is the most effective for determination of urinary arsenic metabolites. Most useful, on-site and in situ analytical methods should be developed.

A Bangladeshi woman pumps water from an untested well. (UNICEF-Bangladesh)

In recent years, some papers were published which report on the generation of monoclonal antibodies for metal ions (for example cadmium and mercury), which is a new dimension. These antibodies were prepared by immunization with corresponding metal-chelator-complex-protein conjugates as immunogens, mainly. So far, no assay is known which can detect arsenic species. It is the aim of this project to prepare and characterize arsenic-conjugates suitable for subsequent immunization of rabbits.
(*Sun Zhe*)

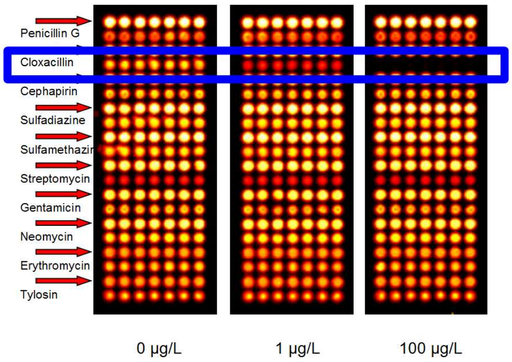
1.3 Bioanalytics II

1.3.1 Development of a Biosensor for the Rapid and Simultaneous Detection of Antibiotics in Milk

Funding: Forschungskreis der Ernährungsindustrie, FEI, FV32ZII
Cooperation: LMU Munich (Prof. Märtlbauer)

The presence of antibiotic residues in milk due to improper use can lead to allergic reactions and the harm of the intestinal flora. There is also concern about increasing bacterial resistance to antibiotics. In the dairy industry, contaminated milk can result in the production problems of cultured products (yoghurt and cheese) due to the inhibition of starter cultures.

Regulatory authorities have established residue limits (MRL) for several antibiotics in bovine milk (EC Regulation 2377/90). Microbial inhibition (e.g., agar diffusion) assays are commonly used as screening tests. One disadvantage of these methods is the duration of about three hours. Usually the results are obtained, when the milk is already in production. For this reason, dairies use quick tests, which can detect the frequently used beta-lactam antibiotics before the milk is pumped out of the dairy van to avoid troubles with fermentation steps in the milk processing. Other antibiotic groups than the beta-lactams cannot be determined with these tests. Furthermore, the dairy has to dispose the whole milk of a diary van in case of a positive test result. To avoid the contamination of the already collected milk, a sensor would be very helpful, which enables the rapid detection of all relevant antibiotics before the milk is pumped into the diary van. The basis for this sensor is the PASA system (Parallel Affinity Sensor Array) which allows the transfer of an indirect ELISA onto a microarray chip. Analyte molecules were immobilized as haptens in an array of spots on a glass slide. The chips were silanized to obtain reactive epoxy groups on the surface. Hapten protein conjugates can bind covalently and by adsorption. The reagents were applied by a non-contact spotting system with a piezo pump. The diameter of the spots was about 350 μm with a spot distance of 0.6 mm. The disposable chip was inserted in a flow cell with a volume of about 100 μL, where all incubations and reactions were carried out automatically. The simultaneous detection of the following analytes is possible in whole milk (detection limits and MRLs in brackets): Penicillin G (3 μg/L, MRL: 4 μg/L), cloxacillin (0.3 μg/L, MRL: 30 μg/L), cephapirin (0.1 μg/L, MRL: 60 μg/L), sulfadiazine (3 μg/L, MRL: 100 μg/L), sulfamethazine (5 μg/L, MRL: 100 μg/L), streptomycin (5 μg/L, MRL: 200 μg/L), gentamicin (10 μg/L, MRL: 100 μg/L), neomycin (30 μg/L, MRL: 1500 mg/L), erythromycin (0.4 μg/L, MRL: 40 μg/L) and tylosin (1 μg/L, MRL: 50 μg/L). Penicillin G could be detected at the maximum residue limit (MRL), the detection limits for all other analytes were far below the respective MRLs. The tests require no sample preparation and can be carried out within 4 minutes 50 seconds. Some assay formats were faster than 3 minutes. For the quantification of samples a calibration with five chips was performed. The test of samples each spiked with several analytes could be demonstrated successfully.

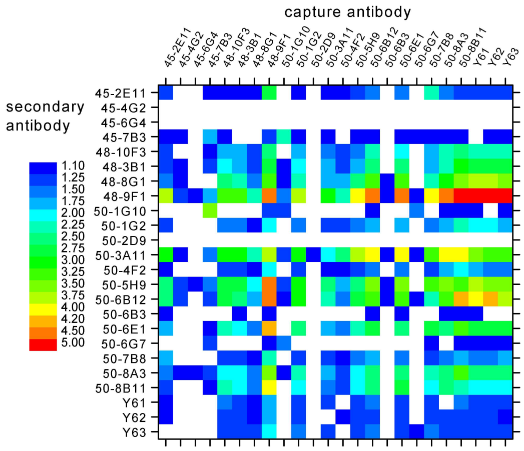


(*B. Knecht*)

1.3.2 Immunoassays for the Detection of Allergenic Contaminations in Food

Funding: EU QLRT-2000-01151
Cooperation: IFA Tulln, Austria (Prof. Krska); RIKILT, The Netherlands (Dr. Haasnoot); Central Science Laboratory, UK (Dr. Banks); r-Biopharm, Germany (Dr. Immer); Università di Milano, Italy (Prof. Restani); Verbruikers Unie, Belgium (S. Mendonça); Central Manchester Hospitals, UK (Dr. Wilson)

Selecting compliant food in the supermarket is still not trivial for people suffering from food allergies. Newspapers and consumer protection magazines often report about incorrectly labeled food. Especially chocolates, cookies and composite products frequently were found to contain allergenic proteins without adequate labeling. On the other hand, excessive precautionary and routine usage of advices on food packages, indicating the potential allergen content, is also not really helpful for allergic patients. Peanut and hazelnut are well known as very critical products. They are used frequently and in great quantities in food industry and contain highly potent allergens. Hazelnut is a major ingredient, e.g. in chocolate, for enhancing the flavor and is contained in nearly all milk chocolates up to a low percent level. Cross-contaminations in factories, where various products are manufactured, therefore are not improbable, for example, when the same production line is used or when peanut/hazelnut dust is transported over the air circulation system.

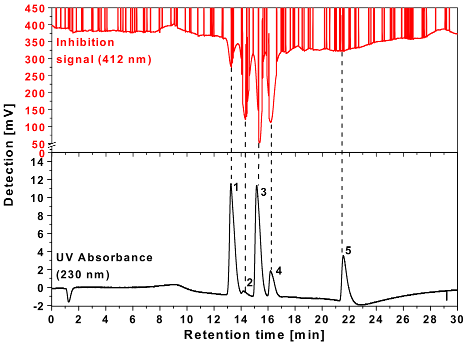


In this project, we developed highly sensitive and selective laboratory-based ELISAs for detecting such hidden allergens in food. Therefore, first of all, numerous antibody pairs were tested (see figure) and the most suitable ones were selected and applied in a sandwich assay. We further optimized and accelerated the tests and so finally could define ELISA protocols with incubation times of 3×10 min, namely sample incubation, incubation of secondary antibody and color development. The ELISAs suitable for rapid screening at a high throughput were validated for cookies, cereals, ice cream, milk chocolate and dark chocolate. Recoveries are ranging from 90% to 110% for most commodities and spiking levels, and the limits of detection, also depending on the matrix, ranged from about 100 ppb to 1 ppm for both peanut and hazelnut. This corresponds to approximately 10-100 ppb peanut/hazelnut protein, respectively. Cross-reactivities were measured for a variety of nuts and seeds and in both assays were found to be in the low ppm range or even not detectable. The ELISAs were applied to numerous commercially available food samples and the results were found to be consistent with data found in literature. In products where peanut/hazelnut was listed as an ingredient, we always found the respective analyte. In case peanut/hazelnut was declared as possibly contained, peanut was only found in few cases, whereas hazelnut was typically found in concentrations from 1.5 ppm up to 1000 ppm. Unfortunately, as expected, we also detected hazelnut in some food samples at a low ppm level, in one particular case even at 5800 ppm, where the allergen declaration was completely missing.
(*M. Kiening*)

1.3.3 Development of a Method for Effect-Related Analysis of Toxins

Funding: BMBF 02WU0331
Cooperation: Institute of Technical Biochemistry (Stuttgart), German Research Centre for Biotechnology (Braunschweig)

Public health departments need to judge the purity of groundwater and surface water for drinking water supply and leisure time activities, preferably by cost-saving and rapid methods. The challenge is to analyse a complex mixture of substances that could be responsible for acute or chronic effects in exposed organisms. The enormous variety of potential contaminants prevents a complete chemical analysis. The determination of unknown toxicants by HPLC separation is tedious due to missing standard substances. The toxicological relevance of the compound is usually assessed by test organisms. Test organisms are mussels, algae, fishes as well as microorganisms as luminescent bacteria. These biotests are not only time consuming, but also of only limited relevance, as singly acute toxicity is detected and the cause of effect often stays hidden. By combining the two powerful techniques of biological assays and liquid chromatography it is possible to develop rapid and cost-efficient detection methods for the requirement of actual environmental analysis. The chemical analysis of contaminants with respect to the biological effects would one allow to assess the hazardous constituents in a complex mixture.



As a first step to a multidimensional effect-related analysis for toxins, an analysis system using HPLC combined with an enzyme-inhibition assay as a biomolecular recognition step was designed. As a model system for neurotoxicity the enzyme acetylcholine esterase is used as the molecular target in the effect-related detection unit. The analytes (spiked insecticide standards) of a water sample are separated with reversed phase chromatography on a C18 column. The column outlet is coupled online to an enzyme inhibition assay, which measures the residual enzyme activity homogenously and continuously. The activity of the enzyme is detected by the Ellman‘s reagent at 412 nm. The elution of potentially toxic substances is observed by a negative signal caused by the reduction of enzyme activity. The sensitivity and selectivity of the enzyme inhibition detector depends largely on the performance of the fluidic system. To reduce peak broadening by longitudinal diffusion and other mechanisms in the reaction tubing, an air segmentation method known from FIA was applied. Insertion of bubbles at high frequency segmented the stream into small reaction volumes and dispersion by the laminar flow decreased. A complex mixture of five insecticides (carbamates, organophosphates and organothiophospates) could be separated with nearly no loss in resolution compared to the UV-detector (see figure).
(*S. Fabel*)

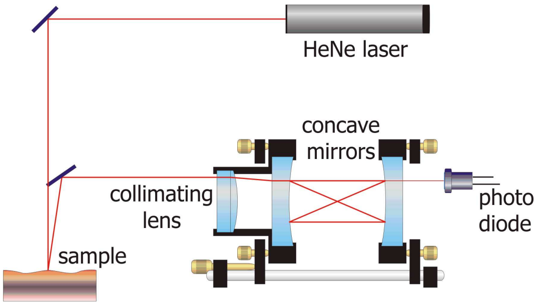
1.4 Applied Laser Spectroscopy

1.4.1 Non-Contact Detection of Optoacoustical Signals

Funding: IWC

Optoacoustic imaging is one of the main interests of the Laboratory for Applied Laser Spectroscopy. The principle of this technique is the conversion of optical pulses in pressure signals by absorption and thermal expansion. The light pulses, created by a pulsed tuneable laser system are delivered to the sample, e.g. the biological tissue. The pressure pulses are detected by piezoelectric sensors and converted in electric signals.

In the framework of a diploma thesis, the possibility of replacing the piezo detector by non-contact interferometry is investigated. The advantage of this technique is a better spatial resolution, as the sensitivity of an optical detection does not directly correlate with the area of the detector. Measurements are possible on samples which are not amenable for direct contact with a sensor, e.g. in medicine and biology.



In the diploma thesis, different types of interferometers were compared theoretically from its key parameters in respect to the measuring task. In order to gain experience with interferometry and to clarify some fundamentals of the instrumentation, a Michelson interferometer was set up and applied on OA model systems.

To achieve a sensitivity comparable to piezo sensors, an other type of interferometer was necessary. A confocal Fabry-Perot interferometer combines extremely small band width with the mechanical robustness necessary for practical applications outside the laboratory. Signal intensities with such instrument exceed the Michelson interferometers by two orders of magnitude. Additionally, an electronic stabilization improves the signal-to-noise-ratio.
(*N. Dudeck*)

1.4.2 Photophoretic Particle Separation

Funding: DFG Ni 261/16-1

For some years, cross-flow separation techniques for the separation of particles and liquid, resp. gaseous media are one major focus at the IWC. Aerosols and colloids are separated by means of thermal and flow fields. Founded by the DFG, the application of electro-magnetic fields, i.e. light, is tested in order to sort particles regarding their optical properties. The project is split into two parts, one dealing with aerosol particles, i.e. microparticles carried by a gas stream, the second one is intended to develop a systems colloid separation similar to the FFF system.

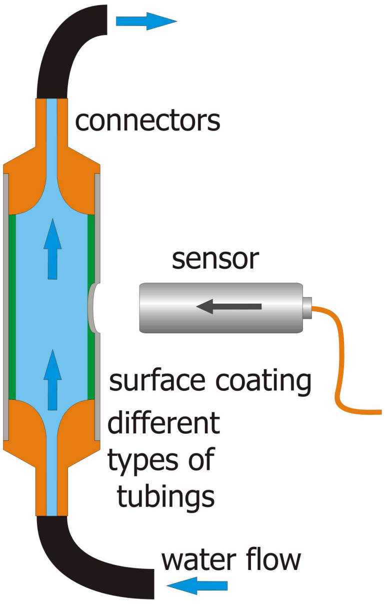
In the aerosol part the particles are sucked with very low velocity through a flow channel. Orthogonally to the flow, a laser beam for illumination is directed through the channel, a second laser can be switched on and off to generate the photophoretic force. A photographic camera observes the aerosol flow and allows in combination with the appropriate image treatment software the calculation of particle trajectories.

Aerosols of different optical properties are compared and mixed and significantly different deflections can be observed.
(*A. Bosniak-Soraja*)

1.4.3 Photoacoustic Sensor Systems for the in-situ Characterisation of Microscalings in Water Conducting Tubes

Funding: IWC

Photoacoustic (PA) or Optoacoustic spectroscopy is applied for many years in various applications. Specially, the characterisation of biofilms and other deposits in aquatic systems is carried out very successfully. Biofilm growth and behaviour can be monitored in situ and depth-resolved. Also, the deposition of inorganic coatings can be observed.



Up to now, most of these PA experiments were realized on glass surfaces of optical prisms. Although these prisms have a special coating to facilitate biofilm growth, there is still a difference to surface coating deposition on normal tubing material as used in industry and civil engineering. Hence, in a project and diploma thesis financed by the institute, PA sensor systems where developed which allow the detection of deposits on any kind of tubing material. These sensors are engineered to measure coating thickness on the untouched surface of a tube.

Two different types were developed and constructed. One is our so-called sensor stick, which is applied through a hole in the tube side. The light is delivered fibre-optically and the detecting piezo foil is fixed concentrically around the fibre. This construction makes a small handy sensor of only 6 mm outer diameter and a length of 10 cm. Disadvantage of the setup is, that absorption of the liquid in the tube influences the optical energy deposited on the surface and, in consequence, leads to artefacts. On the other hand, the system is easy to handle and can be applied for many different types of tubes and other systems.

An alternative sensor is implemented in a clamp, which can be placed around the tube. The clamp contains the piezo sensor, which is pressed against the outer wall of the tube. Laser light is delivered into the tube either by fibre optics or directly via a window opposite to the sensor.
(*M. Janko*)

1.4.4 Microanalysis by Laser-Induced Plasma Spectroscopy (LIPS)

Funding: DFG Pa 716/2-1

Laser-induced plasma spectroscopy (LIPS) is a powerful tool for multielement analysis of solids, liquids, and gaseous samples. For LIPS an intense, pulsed laser beam is focused on the sample of interest, resulting in an evaporation, atomization, and partial ionization of the sample in an expanding plasma cloud. After a delay of some hundred nanoseconds to discriminate against the recombination background, the elemental composition of the sample can be determined via the spectrally and temporally resolved detection of the characteristic atomic and ionic emissions. Due to the minimum sample preparation, the low cost for a single measurement, and the potential for an extensive automation, LIPS is an attractive approach to a fast elemental analysis for many applications.

In this work a LIPS set-up for microanalysis was employed and allowed spatially resolved analysis with a minimum crater size of 20 μm and a nominal depth resolution of 150 nm per pulse. A simultaneous detection with two spectrometers of different wavelength ranges was added to increase the spectral coverage from the VUV to the Vis/NIR range. The integrated VUV echelle permits a full spectral coverage between

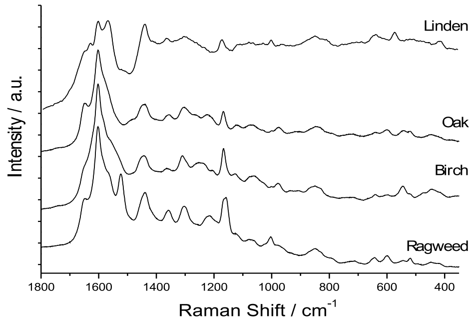
150 and 300 nm with a resolving power between $\lambda/\Delta\lambda$ = 11000 - 15000, while the second external echelle spectrometer covers the wave regions between 200 and 700 nm with a resolution of $\lambda/\Delta\lambda = 10000$. Microanalysis was demonstrated for the quasi non-destructive surface analysis of heat-treated gemstones. Major objective was the detection of Beryllium in the lower ppm-range. The spatial analysis resulted in a good correlation to earlier measurements by laser ablation inductively coupled mass spectrometry (LA-ICP-MS) measurements with a minimal carat loss. The minimal detection, which is estimated to 5.6 ppm Be, allowed the setup of a mobile system for a commercial customer.

In a further application single μm-particles deposited on a filter were analysed. In combination with Raman microscopy, LIPS facilitates the detection and identification of inorganic compounds from clean room samples. The VUV performance of the system was demonstrated for analysis of non-metals in steel. Monitoring of non-metals, such as sulphur, carbon, and phosphorus is one of the essential analytical tasks during steel production. Detection limits for C, S, and P were in the lower ppm range. In this context the LIPS analysis of phosphorylated proteins on blot membranes was studied. Reversible phosphorylation of proteins plays a central role in many biochemical pathways. Hence, LIPS could be a simple and fast method for the detection of phosphorus, carbon and sulfur in phosphorylated proteins. Preliminary work demonstrated the general validity of the approach. However, no quantification could be achieved due to considerable inhomogenities of the blots.
(*M. Müller*)

1.4.5 Characterization and Discrimination of Pollen by Raman Microscopy

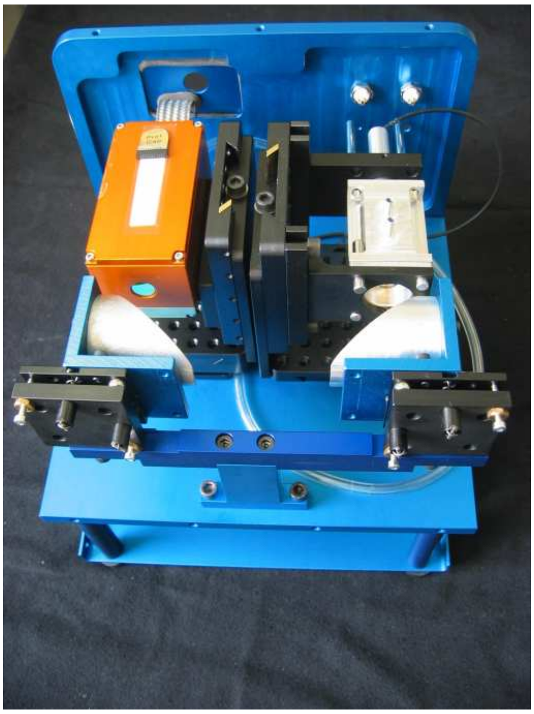
Funding: IWC

The chemical characterization and discrimination of allergy-relevant pollen (ragweed common (Ambrosia artemisiifolia), birch white (Betula pendula), oak English (Quercus robur), and European linden (Tilia cordata)) has been studied by Raman microscopy. Spectra were obtained at different excitation wavelengths (514, 633, 780 nm) and various methods were examined to minimize the strong fluorescence background. The use of He-Ne laser (633 nm) for excitation yields high-quality single pollen Raman spectra, which contain multiple bands due to pollen components such as carotenoids, proteins, nucleic acids, carbohydrates, and lipids. Multivariate classification, i.e. principal component analysis (PCA) and hierarchical cluster analysis, demonstrated the validity of the approach for discrimination between different pollen species.
(*N. P. Ivleva*)



1.4.6 Set-up of a Photoacoustic Demonstrator for Quantification of CO_2

Funding: IWC
Cooperation: TU Vienna, Prof. Lendl



Quantum Cascade Lasers (QCLs) are semiconductor lasers which can be manufactured with literally any emission wavelength between 4 μm and 12 μm. This fact in combination with the simple handling makes it a ideal tool for IR spectroscopy. By means of absorption spectroscopy, a wide range of gaseous compounds can be quantified. A special form of absorption measurement is photoacoustics (PA). It allows the detection the deposed energy, hence giving a measure of the actual absorbed energy, independent on light scattering.

Due to the particular beam profile of a QCL, the setup for PA spectroscopy in combination with QCLs is different from conventional PA setups. In a 4-month study a demonstrator of such instrument for the detection of CO_2 was developed and constructed. A new kind of acoustical resonator, a so-called Helmholtz resonator had to be designed. As the system is intended for routine applications, also the complete opto-mechanical integration had to be optimized for robustness and easy handling. The housing needs to be gas-tight and flushed with nitrogen in order to avoid absorption of the laser energy between the laser housing and the PA cell by atmospheric CO_2.

The intention of this project was to gain experience with QCLs and PA spectroscopy in combination with this laser type, as this combination will is a very promising concept and for sure will be subject of further research of the laser group.

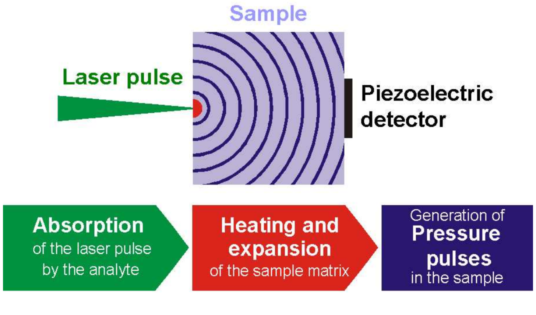
(*C. Haisch*)

1.4.7 Optical Absorption Measurements of Opaque Liquids by Photoacoustic Spectroscopy

Funding: IWC

Online process monitoring is performed often by spectroscopic methods. Conventional absorption or transmission spectroscopy is hampered in many cases by light scattering and the opacity of the samples and is therefore restricted to diluted and filtered samples. Pulsed laser photoacoustic spectroscopy (PAS) allows the measurement of both, small and large absorption coefficients without any kind of sample preparation. This technique is based on the absorption of short laser pulses in a sample, where non-radiative relaxation leads to a local heating of the irradiated volume. Due to thermal expansion of the sample matrix, pressure pulses are generated which can be acquired by ultrasound detectors (e.g. piezoelectric polymer films).

For optimization of the sensor geometry, a photoacoustic sensor cuvette with two detectors based on a piezoelectric PVDF film was developed. The sensors allowed the simultaneous detection of laser-induced pressure waves perpendicularly to and along the laser beam (transmission mode). Comparison of both detection geometries



resulted in an expansion of the dynamic range of more than one order of magnitude when the transmission mode detector was used. By time-resolved detection and evaluation of diverse pressure waves which were generated by a single laser pulse, optical transmission, photoacoustic signal, and speed of sound of liquid samples could be determined simultaneously. Optical transmission measurements are advantageous in low concentrated samples, whereas evaluation of the photoacoustic signal allows the determination of absorption coefficients in the range of approximately 0.1 to 1000/cm. The influence of absorbing or scattering compounds on the signal was investigated using dye solutions and suspensions of TiO_2 particles. For reference analysis, after dilution of the samples conventional UV-Vis spectroscopy was performed. The determination of the speed of sound was verified by use of different solvents and comparison with literature data.

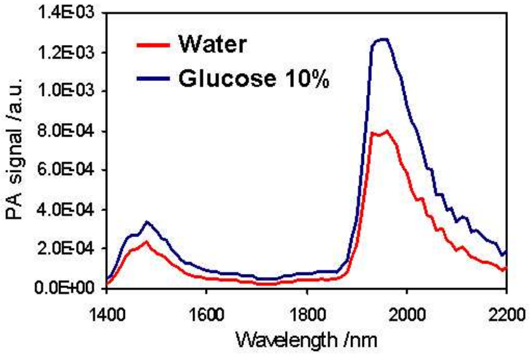
Finally, the optimized sensor geometry was transferred to a photoacoustic flow cell. Laboratory scale experiments demonstrated the potential of this technique in online process control of textile dyeing systems. Textile dye concentrations in the g/L range could be monitored in real time with a temporal resolution of a few seconds.
(*T. Schmid, C. Haisch*)

1.4.8 Near Infrared Spectroscopy of Aqueous Samples using Photoacoustic Detection

Funding: IWC

Near infrared (NIR) spectroscopy of aqueous samples is hampered often by high absorption coefficients of the solvent water. Absorption bands of water – e.g. at 1450 and 1950 nm – cause optical opacity of aqueous solutions or biological samples in this spectral range. Thus, conventional NIR spectroscopy, which is based on the measurement of optical transmission, is restricted to the parts of the NIR range between these water absorptions. This affects for example the determination of sugars in aqueous systems, because several absorption bands of carbohydrates are close to water absorptions in the NIR spectrum.

Since photoacoustic spectroscopy (PAS) is advantageous for the determination of high absorption coefficients (see above), this technique was applied to NIR spectroscopy of aqueous samples. For excitation, a tunable laser system consisting of a frequency-tripled Nd:YAG laser (355 nm) and an optical parametric oscillator (OPO) was employed. This system generates short laser pulses with wavelengths ranging from 410 nm (Vis) up to 2550 nm (NIR). The output wavelength of the OPO was tuned automatically by a LabVIEW software in the range of 1900 to 2300 nm in steps of 10 nm. By use of a flow cell sensor, photoacoustic measurements of aqueous sugar solutions were performed. By evaluation of photoacoustic pressure pulses, NIR absorption spectra of pure water and solutions of saccharose, glucose and fructose with concentrations ranging from 6 to 20% could be determined. In the spectra no saturation effects were observed, even around the strong water absorptions at 1450 and 1950 nm. Simultaneously to the optical absorption, the speed of sound in the sample can be determined by the photoacoustic technique. Experiments showed, that the speed of sound depends linearly on the concentration of saccharose, glucose and fructose, respectively and can be used therefore as an additional parameter for calibration. Additionally, the influence of



temperature on speed of sound and photoacoustic signal was investigated in the range of 4 to 26°C. Here, the measurement values were in good agreement with theoretical predictions.

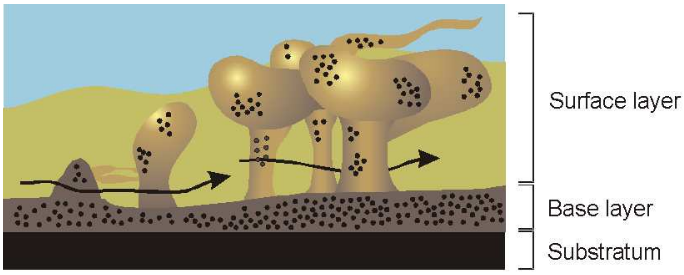
In further experiments, additional spectra will be determined at constant temperature, which will be used as a data basis for the test of different calibration models. Finally, the photoacoustic detection will be transferred to sensor setups for online monitoring of slurries and non-destructive analysis of fruits.
(*T. Schmid*)

1.4.9 Biofilm Monitoring by Photoacoustic Spectroscopy

Funding: DFG Ni 261/14-1,2
Cooperation: Institute of Water Quality Control and Waste Management (TUM)

Additionally to absorption measurements in liquids, photoacoustic spectroscopy allows depth profiling of layered samples. This feature is based on the measurement of time delays between excitation by a laser pulse and detection of pressure waves. If the speed of sound of the sample is known, time delays can be converted into distances. In this way, the depth of an optical absorption event inside the sample can be calculated. This principle was verified by use of well-defined multi-layered samples consisting of polymer films or agar-agar hydrogel layers.

Depth-resolved photoacoustic measurements were applied to on-line and in situ monitoring of biofilms. Biofilms are aggregates of microorganisms which are embedded in a hydrogel formed by extracellular polymer substances (EPS). EPS consist of polysaccharides, proteins and other biopolymers, which are produced by the microorganisms themselves and can contain adsorbed macromolecules from other origins. Biofilms grow on almost every natural surface and are of relevance in some technical processes. Here, the unwanted deposit of biological matter on solid surfaces leads to biofouling. This term summarizes different phenomena, such as the increase of frictional resistance in tubes and pressure differences in membrane processes or the decrease of the heat transfer efficiency of heat exchangers. Additionally, biofilms can clog nozzles and valves and can provide a habitat for pathogenic microorganisms. The most important beneficial application of biofilms are biofilm reactors for wastewater treatment. In such reactors, immobilized bacteria and protozoa are used for degradation of organic and inorganic pollutants. For both, process optimization of wastewater treatment plants and enhancement of biocide efficacy, a nondestructive technique for on-line and in situ analysis of biofilms is necessary.



Photoacoustic spectroscopy allows a non-destructive and depth-resolved on-line monitoring of such microbial aggregates. In this way, the influence of the physico-chemical conditions on structure and stability of biofilms was investigated. Soluble (e.g. acids, bases, biocides or hydrogen peroxide) or particulate substances (e.g. iron oxide particles) were added to the system and changes in density and thickness of the biofilm were monitored by photoacoustic measurements. The influence of flow conditions was investigated by measuring biofilms at different positions inside a flow channel and by changing the flow velocity. Depth-resolved measurements allowed the elucidation of detachment mechanisms (e.g. erosion of small aggregates vs. sloughing off of relatively large areas) and distributions of adsorbed particles inside the film. Current research activities are focused on the investigation of enzymes (e.g. pepsin) which are able to hydrolyze EPS components selectively. Additionally, the interaction between biofilms and surfactants such as SDS was analyzed.

Within the running project, photoacoustic spectroscopy is employed for the first time not only for monitoring of the biofilm itself but also for investigation of mass transport and degradation of pollutants inside microbial aggregates. As model pollutants, biodegradable azo dyes are used which can be determined by photoacoustic measurements in the visible spectral range. First experiments showed, that diffusion of such compounds inside biofilm models consisting of agar-agar hydrogel can be monitored in a depth-resolved fashion.
(*T. Schmid*)

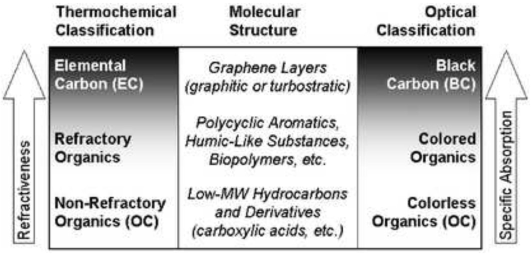
1.5 Aerosol Research

1.5.1 Carbonaceous Aerosol Components: Chemical Composition, Reactivity and Hygroscopicity (CARBAERO)

Funding: BMBF (AFO20000, 7ATC05)

The effects of aerosols on atmospheric chemistry and physics, climate, and human health are among the central topics of current environmental research. Aerosol particles can influence the Earth's energy balance by absorption and scattering of radiation, modify the hydrological cycle by formation of clouds and precipitation, and affect the abundance of trace gases by heterogeneous chemical reactions and other multiphase processes. Moreover, they can cause respiratory, cardiovascular, and allergic diseases when deposited in the human respiratory tract.

The environmental and health effects of aerosols are primarily determined by particle number concentration, size distribution, structure, and chemical composition. Numerous studies have shown that carbonaceous components are major constituents of tropospheric aerosols (10-50% mass fraction), that black carbon is the main light absorber in air particulate matter, and that organics can strongly affect the physicochemical particle properties. The actual composition of atmospheric particles is, however, spatially and temporally highly variable, and the abundance and physicochemical properties of carbonaceous components have been characterized only sparsely and incompletely up to now. Within the project CARBAERO research activities have been pursued and scientific results have been achieved in the following areas:



- Development and optimisation of analytical methods (liquid and solid phase extraction, liquid and gas chromatography, optical spectroscopy and mass spectrometry, enzymatic and immunochemical assays, etc.) for the determination of carbonaceous aerosol components: polycyclic aromatic hydrocarbons; nitrated and oxygenated PAH derivatives; proteins and nitrated derivatives; elemental carbon; cellulose, humic-like substances, and water-soluble organic carbon.

- Aerosol field measurements and sampling at urban, rural, and high-alpine locations (Munich, Hohenpeissenberg, Schneefernerhaus/Zugspitze): detection of high protein concentrations (up to 7% of PM2.5); characterisation of PAH filter sampling artefacts (up to 100%; linear correlation with ambient ozone); detection of nitro-PAH in a high alpine clean air environment; observation of characteristic local differences and seasonal trends of aerosol physical properties and chemical composition.

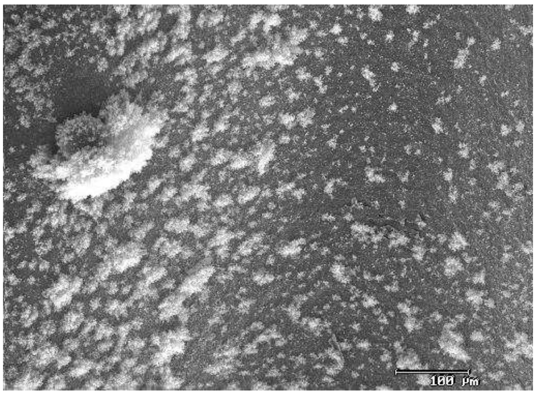
- Experimental investigation and mathematical modelling of the interaction of aerosol particles and components (soot/PAH, proteins) with reactive trace gases (O_3, NO_2) and water vapor: identification of previously unknown PAH nitration and oxidation products ; detection of efficient protein nitration by polluted air and synthetic gas mixtures; deconvolution of adsorption and surface reaction processes and determination of adsorption equilibrium and reaction rate parameters for O_3, NO_2, and H_2O on soot/PAH; development of a kinetic model framework for aerosol surface reactions and gas-particle interactions.
- Experimental investigation and mathematical modelling of the interaction of water vapor with aerosol particles of complex chemical composition (mixtures of salts and biopolymers, etc.): electric charge effects and microstructural rearrangements; phase transitions and hygroscopic growth; kinetic limitation of deliquescence and water uptake by protein envelopes; parameterisation of the practical osmotic coefficient for globular macromolecules.

The results have been presented and discussed in multiple conference contributions and journal articles, and further publications are in preparation.
(*T. Fehrenbach, T. Franze, E. Mikhailov, U. Schaller, C. Schauer, A. Zerrath, U. Pöschl*)

1.5.2 Development of a Filterless Catalytic System for the Continuous Oxidation of Soot Particles for Heavy Duty Vehicles (PM-KAT®)

Funding: Bayer. Forschungsstiftung
Cooperation: MAN Nutzfahrzeuge AG, Nürnberg; Oberland-Mangold, Eschenlohe; Fritz-Haber-Institut, Department of Inorganic Chemistry, Berlin; Max-Planck- Institute for Polymer Research, Mainz

Since conventional soot particle filter systems significantly increase exhaust gas back pressure and are easily clogged by engine oil ashes, current research activities focus on the development of filterless soot particle deposition structures. With the experimental and theoretical support in the framework of this project, the PM-Kat® system could successfully be transferred into serial production. The project work focuses on four major topics:



Investigation of the relevant soot particle deposition mechanisms Optimization of particle deposition and soot storage behaviour of the catalyst structures Investigation of the oxidation kinetics of different kinds of soot under realistic exhaust gas conditions Development of a phenomenological model to reliably predict the governing processes simultaneously

For the investigation of soot particle deposition and oxidation processes a test gas bench with specially designed flat bed reactors has been constructed. With a cross section of 10 × 6 mm these reactors can be flexibly equipped with dfferent types of deposition structures (max. length 290 mm). The system can be operated at temperatures up to 600 °C with variable gas composition and space velocities of 10,000 - 600,000/h.

Model soot aerosols are produced with a spark discharge generator (graphite electrodes), with a modified LaMer-Sinclair generator (polycyclic aromatic hydrocarbons, e.g. hexabenzocoronene) or a light duty vehicle diesel engine in combination with aerosol conditioning measures. Aerosol particle number size distributions before and after the deposition device are measured with an scanning mobility particle sizer (SMPS) system consisting of an electrostatic classifier and a condensation particle counter (CPC). Mass based soot deposition efficiencies are determined with the photoacoustic soot sensor (PASS) allowing a time resolution of 5 Hz. Sophisticated temperature control devices have been implemented to ensure isothermal sampling conditions at all sampling points and to minimize potential measurement artefacts due to thermophoretic sampling losses.

Numerous catalyst structures have been characterized with respect to transient and stationary particle deposition effciencies under varying flow and temperature conditions, and particularly efficient deposition was observed for steel-structures coated with microspheres (50 to 150 μm diameters, see Figure). The optimization of the structures' flow patterns was obtained by computational fluid dynamics (CFD). The contribution of thermophoresis during transient operation of the system was found to have a signficant influence on particle deposition.

The reaction products and kinetics of the oxidation and volatilisation of deposited soot particles (real diesel soot, spark discharge soot, hexabenzocoronene) by nitrogen oxides, oxygen and water have been characterised for a wide range of conditions (temperature, gas composition, space velocity), using FTIR spectroscopy and complementary analytical techniques. A detailed analysis and mechanistic interpretation of the kinetic data shows the significant contribution of sorption processes to the overall soot reaction rates.
(*C. Adelhelm, A. Messerer, D. Rothe, A. Thalhammer*)

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M. Lackhoff und R. Nießner; Schadstoffabbau durch UV-Strahlung. Rundgespräche der Kommission für Ökologie 27 (2004) 149-154

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D. Su, R. Jentoft, J.-O. Müller, D. Rothe, E. Jacob, C. Simpson, K. Müllen, A. Messerer, U. Pöschl, R. Niessner and R. Schlögl; Microstructure and Oxidation Behaviour of EURO IV Diesel Engine Soot: A Comparative Study with Synthetic Modell Soot Substances. Catalysis Today 90 B (2004) 127-132

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T. Schmid, U. Panne, J. Adams and R. Niessner; Investigation of Biocide Efficacy by Photoacoustic Biofilm Monitoring. Water Research 38 (2004) 1189-1196

C. Schauer, R. Niessner and U. Pöschl; Analysis of Nitrated PAHs by LC with Fluorescence and MS Detection: Soot, Air Particulate Matter, and Reaction Product Studies. Anal. Bioanal. Chem. 378 (2004) 725-736

R. von Kuhlmann, M. G. Lawrence, U. Pöschl, P. J. Crutzen, Sensitivities in Global Scale Modeling of Isoprene, Atmospheric Chemistry and Physics, 4 (2004) 1-17.

2.2 Journal articles (non-reviewed)

C. Adelhelm, C., R. Niessner, U. Pöschl, Generation, Characterization and Oxidation of Ultrafine Hexabenzocoronene Particles, Journal of Aerosol Science (2004), 35, S173-S174.

R. Forkel, B. Bonn, R. von Kuhlmann, E. Haas, H. Geiger, I. Barnes, U. Pöschl, Validation of Chemical Mechanisms for the Description of Isoprene and Alpha-Pinene Degradation Within 3-Dimensional Chemistry-Transport Models (VALCHEM), AFO2000 Newsletter, 9 (2004) 3-6.

A. Messerer, R. Niessner, U. Pöschl, Continuous Soot Particle Deposition and Oxidation in Novel Particle Trapping Oxidation Catalysts, Journal of Aerosol Science, 35 (2004) S1185-S1186.

U. Pöschl, U., Interactive Journal Concept for Improved Scientific Publishing and Quality Assurance, Learned Publishing, 17 (2004) 105-113.

U. Pöschl, S. Bhowmik, T. Fehrenbach, T. Franze, E. Mikhailov, U. Schaller, C. Schauer, A. Zerrath, Carbonaceous Aerosol Components: Composition, Reactivity, and Hygroscopicity (CARBAERO), Journal of Aerosol Science, 35 (2004) S343-S344.

A. Strasser, B. G. Knecht, M. G. Weller, R. Niessner, R. Dietrich and E. Märtlbauer; Microarray-System zum Nachweis von antimikrobiellen Rückständen in Milch, GIT Laborfachzeitschrift 48(9) (2004) 831-834.

2.3 Monographs

D. Knopp and R. Niessner; Biomonitors Based on Immunological Principles. In: Solid Waste: Assessment, Monitoring and Remediation (Eds.: T. Twardowska, H. E. Allen, A. A. F. Kettrup, W. J. Lacy) Elsevier Science B.V. Amsterdam, (2004) 505-537.

M. G. Weller; Protein Microarrays for Biosensor Applications, in: Protein Microarrays, M. Schena (Ed.), Jones & Bartlett Publ., Boston (2004) 285-303.

2.4 Conference Presentations

2.4.1 Oral Presentations

M. Alte, C. Radl, R. Niessner & T. Baumann, Mobility and Kinetics of Dissolved CO_2 in Calcareous Pore Aquifers, EGU, 1st General Assembly, 26.–30.4.2004, Nice.

T. Baumann & C. J. Werth, Identifying Colloid-Matrix Interactions at the Pore Scale, EGU, 1st General Assembly, 26.–30.4.2004, Nice.

T. Baumann, N. Nestle & R. Niessner, MRI to Investigate Dynamic Subsurface Processes, Interfaces Against Pollution 2004, 24.–27.5.2004, Jülich.

T. Baumann, M. Alte, C. Radl & R. Niessner, Mobilität und Gleichgewichtskinetik von gelöstem CO_2 in einem carbonatischen Grundwasserleiter, FH-DGG Tagung, 19.–22.5.2004, Darmstadt.

A. Messerer, U. Pöschl, R. Niessner, H.-J. Schmid, C. Knab, Erhöhung der Abscheidung ultrafeiner Dieselrußpartikeln durch Mikrokugelbeschichtung auf metallträgerbasierten Katalysatorstrukturen, GVC Fachausschusssitzung "Gasreinigung", 16.–17.2.2004, Karlsruhe.

A. Messerer, R. Niessner, U. Pöschl, Continuous Soot Particle Deposition and Oxidation in Novel Particle Trapping Oxidation Catalysts, European Aerosol Conference, 6.–10.9.2004, Budapest.

A. Messerer, U. Pöschl, R. Niessner, Investigations on Novel Particle Trapping and Oxidation Catalysts for the Continuous Removal of Diesel Particulate Matter, 8th International Conference on Carbonaceous Particles in the Atmosphere, 14.9.–16.9.2004, Vienna.

N. Nestle, A. Wunderlich & T. Baumann, MRT-Langzeituntersuchungen zur Ausbreitung von Kolloiden und Schwermetallionen in statischen Lockersedimenten, FH-DGG Tagung, 19.–22.5.2004, Darmstadt.

R. Nießner, A Novel Approach for the Continuous Deposition and Oxidation of Diesel Particulate, Carbon Aerosol Conference, 15.9.2004, Wien

R. Nießner, A Novel Approach for the Continuous Deposition and Oxidation of Diesel Particulate, American Association for Aerosol Research Conference, 4.10.2004, Atlanta

U. Pöschl, S. Bhowmik, T. Fehrenbach, T. Franze, E. Mikhailov, U. Schaller, C. Schauer, A. Zerrath, Carbonaceous Aerosol Components: Composition, Reactivity, and Hygroscopicity (CARBAERO), AFO2000 Final Seminar, 22.–24.3.2004, Bad Tölz.

U. Pöschl, S. Bhowmik, T. Fehrenbach, T. Franze, E. Mikhailov, U. Schaller, C. Schauer, A. Zerrath, Carbonaceous Aerosol Components: Composition, Reactivity, and Hygroscopicity (CARBAERO), European Aerosol Conference, 6.–10.9.2004, Budapest.

U. Pöschl, Zusammensetzung und Transformation kohlenstoffhaltiger Aerosolkomponenten, TROPEIS II Workshop, 10.–11.11.2004, Frankfurt.

U. Pöschl, Y. Rudich, M. Ammann, Kinetic model framework for aerosol surface chemistry and gas-particle interactions: general equations and terminology, ACCENT Workshop, 13.–14.12.2004, Cambridge.

2.4.2 Poster Presentations

C. Adelhelm, R. Niessner, U. Pöschl, Generation, Characterization and Oxidation of Ultrafine Hexabenzocoronene Particles, European Aerosol Conference, 6.–10.9.2004, Budapest.

B. Bonn, von Kuhlmann, R., M. G. Lawrence, U. Pöschl, Validation of Chemical Mechanisms for the Atmospheric Degradation of Isoprene and -Pinene - Global Modelling Including SOA Formation, AFO2000 Final Seminar, 22.–24.3.2004, Bad Tölz.

O. Fenton, R. Niessner & T. Baumann, Development of a high throughput test design for the determination of sorption parameters of aquifer materials, Wasserchemische Gesellschaft, 17.–19.5.2004, Bad Saarow.

S. Maier, R. Niessner, M. G. Weller; Aufbau einer wirkungsbezogenen Analysenmethode mit Acetylcholinesterase als Modelltarget, Wasserchemische Gesellschaft, 17.–19.5.2004, Bad Saarow.

D. Matschulat, A. Deng, J. Lai, R. Niessner, D. Knopp; Analytical tools for the determination of benzo[a]pyrene in drinking water: new natural and artificial antibodies, Wasserchemische Gesellschaft, 17.–19.5.2004, Bad Saarow.

A. Messerer, D. Rothe D., C. Knab, U. Pöschl, R. Niessner, New Strategies for Particulate Emission Reduction of HD Vehicles, 8th International ETH-Conference on Combustion Generated Nanoparticles 2004, 16.–18.8.2004, Zurich.

A. Messerer, V. Schmatloch, U. Pöschl , R. Nießner, Simultane Wärmeübertragung und Partikelabscheidung - ein neuer Ansatz zum effizienten Betrieb von Kleinfeuerungsanlagen, DECHEMA/GVC-Jahrestagung 2004, 12.–14.10.2004, Karlsruhe.

U. Pöschl, S. Bhowmik, T. Fehrenbach, T. Franze, E. Mikhailov, U. Schaller, C. Schauer, A. Zerrath, Carbonaceous Aerosol Components: Composition, Reactivity, and Hygroscopicity, EGU General Assembly 2004, 25.–30.4.2004, Nice.

U. Pöschl, S. Bhowmik, T. Fehrenbach, T. Franze, E. Mikhailov, U. Schaller, C. Schauer, A. Zerrath, Carbonaceous Aerosol Components: Composition, Reactivity, and Hygroscopicity (CARBAERO), European Aerosol Conference, 6.–10.9.2004, Budapest.

U. Pöschl, T. Fehrenbach, T. Franze, E. Mikhailov, U. Schaller, C. Schauer, A. Zerrath, Chemical Transformation and Water Interaction of Carbonaceous Aerosol Components, 8th International Conference on Carbonaceous Particles in the Atmosphere, 14.–16.9.2004, Vienna.

Prestel, H., Schott, L., Nießner, R. und Panne, U.: Charakterisierung von Kläranlagen-Kolloiden mittels AF4/ICP-MS, Wasserchemische Gesellschaft, 17.–19.5.2004, Bad Saarow.

T. Schmid, U. Panne, C. Haisch, R. Nießner: Laserinduzierte photoakustische Spektroskopie als Sensorprinzip: Anwendungen in der Prozess- und Umweltanalytik, Wasserchemische Gesellschaft, 17.–19.5.2004, Bad Saarow.

2.4.3 Invited Lectures

T. Baumann, Transportprozesse im Grundwasserleiter – Vom Feldversuch zur Porenskala und zurück, Institut für Geowissenschaften, TU Darmstadt, 9.6.2004, Darmstadt.

T. Baumann, Transport on the Microscale, Zentrum für Angewandte Geowissenschaften, Univ. Tübingen, 19.11.2004, Tübingen.

C. Haisch, Photoakustische Spektroskopie: Grundlagen und Anwendungen, 14.5.2004, TU Wien.

C. Haisch, Dynamic Online Particulate Measurement, 3. International Exhaust Gas and Particulated Emissions Forum, 14.–15.9.2004, Sinsheim.

D. Knopp, Selective Analyte Enrichment with Antibodies and Molecularly Imprinted Polymers (MIPs), 11th Symposium on Sample Handling for Environmental and Biological Analysis, 18.–21.4.2004, Baiona/Pontevedra, Spain.

D. Knopp, Preparation of Immunoaffinity Columns for Sample Cleanup and Their Applicability to the Analysis of Sulfonylurea Herbicides. ExTECH 2004, 6.-8.9.2004, Leipzig.

R. Nießner, Photokatalytischer Schadstoffabbau an Partikeln, Bayer. Akademie der Wissenschaften, 9.2.2004, München.

R. Nießner, Neues zur Dieseabgasreinigung (Partikel) und Online-Messung, PALAS Workshop, 10.2.2004, Wörth.

R. Nießner, Future Trends & Challenges in Analytical Chemistry, National University of Singapore, Dept. of Chemistry, 4.3.2004, Singapore.

R. Nießner, On-line & In Situ Chemical Analysis of Organic Aerosol, Desert Research Institute, 3.4.2004, Las Vegas.

R. Nießner, Characterisation of Soot Aerosol: Thermal Analysis vs. Light Interaction, Environmental Protection Agency, 9.4.2004, Research Triangle Park.

R. Nießner, Sampling for Environmental Process Analysis, EUROANALYSIS, 6.9.2004, Salamanca.

R. Nießner, Future Trends & Challenges in Analytical Chemistry, EUROANALYSIS, 8.9.2004, Salamanca.

R. Nießner, Future Trends & Challenges in Analytical Chemistry, Merck, 10.9.2004, Darmstadt.

R. Nießner, Laser or Antibodies – Best Friends of Analysts, National Meeting of Italian Analysts, 20.9.2004, Parma.

R. Nießner, Future Trends & Challenges in Analytical Chemistry. 26.11.2004, Universität Mainz

U. Pöschl, Tropospheric Aerosols: Particle Properties, Transformations and Water Interactions, Institute for Atmospheric and Climate Research, 26.1.2004, ETH Zürich.

U. Pöschl, Aerosolzusammensetzung, Partikelstruktur, und Gas-Partikel-Wechselwirkungen, Institut für Strahlenschutz, GSF Forschungszentrum, 17.3.2004, München.

U. Pöschl, Carbonaceous Aerosol Components: Composition, Reactivity, and Hygroscopicity, AFO2000 Final Seminar, 22.3.2004, Bad Tölz.

U. Pöschl, Open Access: Scientific Quality Assurance by Interactive Peer Review and Public Discussion, 68. Physikertagung der Deutschen Physikalischen Gesellschaft, 23.3.2004, München.

U. Pöschl, Atmospheric Aerosol Composition, Particle Structure, and Gas-Particle Interactions, Institute for Meteorology and Climate Research, 26.4.2004, Forschungszentrum Karlsruhe.

U. Pöschl, Atmospheric Aerosol Properties and Processes, Institute for Marine and Atmospheric Research, 7.4.2004, Utrecht University.

U. Pöschl, Physical and Chemical Transformation of Biological and Combustion Aerosol Particles, IGAC-ILEAPS-SOLAS Workshop on Organic Aerosols and Global Change, 10.5.2004, Hyytiälä.

U. Pöschl, New Models of Open Access E-Publishing and Scientific Quality Assurance: a Scientist's Perspective, The Digital Library and e-Publishing for Science, Technology, and Medicine, CERN, 15.6.2004, Geneva.

U. Pöschl, Atmospheric and Climate Research, Institute of Physical Chemistry, 21.6.2004, University of Bielefeld.

U. Pöschl, Experimental Investigation and Mathematical Description of Surface Reactions, Telluride Workshop on Atmospheric Aerosol Aging, 10.8.2004, Telluride.

U. Pöschl, K. S. Carslaw, T. Koop, R. Sander, W. T. Sturges, J. P. D. Abbatt, J. T. Jayne, D. R. Worsnop, Scientific Quality Assurance by Interactive Peer Review and Public Discussion, 228th American Chemical Society National Meeting, 22.8.2004, Philadelphia.

U. Pöschl, Why and How Shall Open Access Publishing Improve Scientific Communication and Quality Assurance?, US National Research Council and National Academy of Sciences, 25.10.2004, Washington DC.

U. Pöschl, Composition, Reactivity, and Water Interactions of Carbonaceous Aerosol Components, Max-Planck-Institut für Chemie, 12.11.2004, Mainz.

U. Pöschl, Kohlenstoffhaltige Aerosole: Chemische Zusammensetzung und Reaktivität, DBG-DECHEMA-GDCh Gemeinschaftsausschuss für Chemie der Atmosphäre, 16.11.2004, Frankfurt.

U. Pöschl, Oxidation und Nitrierung von Ruß, polyzyklischen Aromaten und Proteinen, DECHEMA-Expertengespräch Dieselrußpartikelfilter und Luftqualität, 30.11.2004, München.

M. G. Weller, Parallel Affinity Sensor Arrays as a Tool for Immunological Multianalyte Detection", 2nd International Workshop on Multianalyte Biosensing Devices, 19.2.2004, Tarragona, Spain.

M. G. Weller, Vorkommen und Analytik von Algentoxinen, Arbeitsgruppe Analytik von Stoffen in der Landwirtschaft - SKLW, 7.6.2004, Dortmund.

M. G. Weller, Arbeitsbereiche der AG Weller am Institut für Wasserchemie der TU München, Fachgruppe Anthropogene Stoffe im Wasserkreislauf - Pharmaka, endokrin wirksame Verbindungen, Hessenwasser, 17.6.2004, Darmstadt.

M. G. Weller, Entwicklung und Anwendung immunologischer Methoden für umweltanalytische, lebensmittelchemische und diagnostische Problemstellungen, Bundesanstalt für Materialforschung und -prüfung (BAM), 12.11.2004, Berlin.

M. G. Weller, Microarrays zur Analyse von Pflanzenschutzmitteln, 57. Fachtagung des Bayerischen Landesamtes für Wasserwirtschaft - Pflanzenschutzmittel und Gewässer, 17.11.2004, München.

2.4.4 Scientific Committee

T. Baumann, EGU, 1st General Assembly, 26.–30.4.2004, Nice; Session Convener.

R. Nießner, Desert Research Institute, Intern. Workshop on Organic Speciation in Athmospheric Aerosol Research, 5.–7.4.2004, Las Vegas; Topic Leader.

2.5 Hydrogeological Consulting

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

Hydrogeological and hydrochemical expertises (mineral water, spa water) Bad Gögging, Bad Brückenau, Hölle, Sibyllenbad, Siegsdorf.

2.6 Bachelor Theses

Ferdinand Haller, Bachelor (Biochemistry): Entwicklung eines Verfahrens zur wirkungsbezogenen Analytik von cyanobakteriellen Toxinen

Ulf Dettmer, Bachelor (Molecular Biotechnology): Untersuchung von Nussproteinen mit immunchemischen und chromatographischen Methoden

2.7 MS and Diploma Theses

MS Pooja Bajaj (Industrial Chemistry): Optimization of Immunochemical Methods for the Rapid Detection of Antibiotics in Milk

Dipl.-Chem. Sabine Bräu (Chemie): Entwicklung einer Multianalyt-HPLC-Methode zur Bestimmung von Antibiotika in Kuhmilch

Dipl.-Chem. Maria Eiberle (Chemie): Optimierung eines microarraybasierten Sensorsystems für die Detektion von Antibiotika in Milch

Dipl.-Geol. Christoph Radl (Geologie): Ausbreitungsverhalten reaktiver Gase in einem durch hohe pH-Werte gekennzeichneten, carbonatischen Grundwasserleiter

Dipl.-Chem. Maria Taige (Chemie): Immobilisierung von biochemischen Reagenzien in Sol-Gel-Kügelchen für die Analyse von cyanobacteriellen Toxinen

Dipl-Ing. Astrid Thalhammer (Chemieingenieurwesen): Experimentelle Untersuchung und Modellbildung zum Oxidationsverhalten von Real- sowie Modellrußen auf neu entwickelten Katalysatorträgerstrukturen

2.8 PhD Theses

Dipl.-Chem. Christian Schauer: Analyse und Reaktivität von PAHs in Aerosolen

Dipl.-Chem. Thomas Franze: Analyse und Reaktivität von Proteinen in atmosphärischen Aerosolen und Entwicklung neuer Immunoassays zur Messung von Nitroproteinen

Dipl.-Phys. Igor Radivojevic: Spectrochemical Analysis of Solid Samples by Laser-induced Plasma Spectroscopy

Apothekerin Bitterle: Oxidative und inflammotorische Mechanismen von Targetzellen des Alvedarepithels nach Exposition mit ultrafeinen Aerosolpartikeln an der Luft-Medium-Grenzschicht

LM-Chem. Petra Degelmann: Entwicklung immunologischer, chromatographischer und massenspektrometrischer Methoden zur Bestimmung von Sulfonylharnstoffen

3 Teaching, Colloquia, and Other Activities

3.1 Classes

Chemie gelöster und ungelöster Wasserinhaltsstoffe, Teil 1: Wasserkreislauf und Gleichgewichte	Nießner
Chemie gelöster und ungelöster Wasserinhaltsstoffe, Teil 2: Hydrokolloide, micellare Systeme und photochemische Umsetzungen	Nießner
Organische Spurenanalytik für Geowissenschaftler	Nießner
Spurenanalytische Techniken	Nießner, Panne, Weller
Umweltanalytik, Teil 1: Grundlagen der instrumentellen Analytik von Wasserinhaltsstoffen	Nießner
Umweltanalytik, Teil 2: Charakterisierung von Luftinhaltsstoffen (Gase und Aerosole)	Nießner
Umweltanalytik, Teil 3: Organische Spurenanalytik an Umweltmatrices	Nießner
Water Chemistry (GIST/NUS Singapur)	Nießner
Aerosolcharakterisierung	Nießner
Einführung in das hydrogeologische Praktikum I, II, III	Baumann, Nießner
Hydrogeologie I und II	Baumann
Ausbreitung von Schadstoffen im Untergrund	Baumann
Erkundung und Sanierung von Grundwasserschadensfällen	Baumann
Modellierung der Grundwasserströmung und des Stofftransports	Baumann
Hydrochemische Modellierung	Baumann
Biochemische und molekularbiologische Analysenverfahren in der Umweltanalytik	Knopp
Gasmesstechnik	Pöschl
Atmosphärenchemie und Klimaforschung (TU Wien)	Pöschl
Kopplungstechniken in der Instrumentellen Analytik	Weller
Massenspektrometrie in der Umweltanalytik	Weller

3.2 Lab Courses and Seminars

Vertiefungsfach Analytische Chemie, Teil 1 Organische Spurenanalytik	Nießner, Weller, Knopp
Teil 2 Methoden der Strukturaufklärung und Instrumentellen Analytik	Nießner und Mitarbeiter, Dozenten in Garching
Wasserchemisches Praktikum I: Wasseranalyse	Knopp, Weller, Nießner
Wasserchemisches Praktikum II: Wassertechnologie	Knopp, Nießner, Weller, Haisch, Knopp
Praktikum Umweltmesstechnik	Pöschl, Nießner, Messerer
Hydrogeologisches Praktikum I: Gesteinsphysikalische Methoden	Baumann, Nießner
Hydrogeologisches Praktikum II: Hydrochemische Methoden	Baumann, Nießner
Hydrogeologisches Praktikum III: Geländeübungen mit Kurs	Baumann, Nießner
Hydrogeologische und hydrochemische Exkursionen	Baumann, Nießner
Hydrogeologisches, hydrochemisches und umweltanalytisches Seminar	Baumann, Nießner

3.3 Institute Colloquia

Prof. Dr. Frank Bier, Universität Potsdam & Fraunhofer-Institut für Biomedizinische Technik: Biochips for Medical Diagnostics (17.1.2004)

Prof. Dr. Gary Amy, Dept. of Civil, Environmental and Architectural Engineering, University of Colorado-Boulder: Chemistry of Natural Organic Matter (22.1.2004)

Prof. Dr. Wolfgang Schuhmann, Analytische Chemie - Elektroanalytik & Sensorik, Ruhr-Universität Bochum (26.1.2004)

Dr. Rainer Meckenstock, Institut für Grundwasserökologie, GSF Neuherberg: Nachweis von natürlichen Selbstreinigungsprozessen im Grundwasser am Beispiel des anaeroben Abbaus von aromatischen Kohlenwasserstoffen (24.3.2004)

Prof. Dr. Silvia E. Braslavsky, Max-Planck-Institut für Bioanorganische Chemie, Mülheim a.d. Ruhr: Time-resolved Thermodynamic Profile in Biological Photosensors (13.4.2004)

Prof. Dr. Bernhard Welz, Departamento de Chimica, Universidade Federal de Santa Caterina, Florianopolis/Brasilien (12.5.2004)

Prof. Dr. Peter Hering, Institut für Lasermedizin, Universität Düsseldorf: Analytischer, diagnostischer und therapeutischer Einsatz des Lasers in Medizin und Life Science (19.5.2004)

Dr. Klaus D.A. Wendt, Institut für Physik, Universität Mainz: Selektive Bestimmung von Ultraspurenisotopen mit resonanter Laser-Massenspektrometrie (2.6.2004)

Prof. Dr. Hubert van den Bergh, Swiss Federal Institute of Technology, Lausanne: Photonics for Early Detection and Treatment of Disease: 3 Examples taken from Fundamentals to the Market (15.6.2004)

Prof. Dr. Martin Frenz, Institut für Angewandte Physik, Universität Bern: Vergleich unterschiedlicher Drucksensoren für optoakustische Bildgebung und Gewebecharakterisierung (25.6.2004)

Dr. Georg Rößling, Pharmazeutische Entwicklung, Schering AG, Berlin: Nanotechnology for the Pharmaceutical Industry (19.7.2004)

Prof. Dr. Achim Wixforth, Experimentalphysik I, Universität Augsburg und Advalytix AG, Brunnthal: Akustisch getriebene fluidische Prozessoren für biologische und chemische Anwendungen im Nanoliterbereich (29.7.2004)

Prof. Dr. Volker Schurig, Institut für Organische Chemie, Universität Tübingen: Enantiomeranalytik durch Kapillar-Chromatographie (31.8.2004)

Dr. Jörg Eppinger, Department für Chemie, TU München: Enzyme Microarrays for Inhibitor Discovery (9.11.2004)

Prof. Dr. Pierluigi Reschiglian, Dept. Chemistry "G. Ciamician", University of Bologna: Field-Flow-Fractionation: The Best-kept Secret in Life Science Separations (14.12.2004)

3.4 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. Dietmar Knopp

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

PD Dr. Ulrich Panne

Spectrochimica Acta B	Advisory Board Member

Dr. Ulrich Pöschl	
Atmospheric Chemistry and Physics European Geosciences Union	Chief Executive Editor President of Atmospheric Sciences Division, Council 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 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)

4.2.2 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
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 chromatographie 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

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 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)

5 Staff 2004

Univ.-Prof. Dr. Reinhard Nießner

Dr. Thomas Baumann
Dr. Swati Bhowmik (until 2/04)
Dipl.-Geogr. Käte Effenberger (until 5/04)
Dr. Christoph Haisch
Dr. Natalia Ivleva
Dr. Dietmar Knopp
Dr. Ulrich Panne (until 8/04)
Dr. Ulrich Pöschl
Dr. Harald Prestel
Dr. Thomas Schmid
Dr. Michael G. Weller

Birgit Apel
Günter Dollinger
Roswitha Glunz
Karin Koller
Joachim Langer
Ramona Leube
Susanne Mahler
Christine Sternkopf
Christa Stopp
Sebastian Wiesemann

Hatice Hazir
Mira Kolar

PhD Students

Dipl.-Chem. Christoph Adelhelm (until 8/04)
Dipl.-Geol. Matthias Alte
Dipl.-Ing. Jackelyn Arágon-Gómez (from 8/04)
Leb.-Chem. Petra Degelmann (until 7/04)
Dipl.-Chem. Susanne Fabel, geb. Maier
Dipl.-Chem. Tobias Fehrenbach
Dipl.-Geol. Owen Fenton (until 6/04)
Dipl.-Leb.Chem. Martin Kiening
Dipl.-Chem. Bertram Knecht (until 6/04)
Dipl.-Chem. Diana Matschulat
Dipl.-Chem. Ulrike McKeon, geb. Schaller
Dipl.-Ing. Armin Messerer
Dipl.-Chem. Dieter Rothe
Dipl.-Geol. Dagmar Spangenberg (until 8/04)

External PhD Students

Apothekerin Ellen Bitterle (GSF) (until 7/04)
Dipl.-Chem. Michael Harris (OMG AG, Hanau)
Dipl.-Biol. Roman Radykewicz (GSF)
Leb.-Chem. Michael Rampfl (IBP Holzkirchen)

Diploma Students/MS Students

Pooja Bajaj (until 1/04)
Ana Bosnjak-Zoraja (from 9/04)
Sabine Bräu (until 2/04)
Wei Chen (from 8/04)
Nikola Dudeck, geb.Heimpel (from 1/04)
Maria Eiberle (3/04 – 11/04)
Marek Janko (until 8/04)
Deepak Kamble (from 7/04)
Gerogos Kassotakis (Erasmus student from Univ. Athens, Greece) (from 9/04)
Maike Müller (from 6/04)
Christoph Radl (until 2/04)
Maria Taige (until 5/04)
Astrid Thalhammer (until 6/04)
Fotios Tsagkogeorgas (Erasmus student from Univ. Athens, Greece) (from 9/04)
Markus Wiesmeier (from 8/04)
Sun Zhe (GIST/Singapore) (from 8/04)

Guests and Research Fellows

Dr. Anping Deng, Sichuan University, Chengan (China) (until 8/04)
Dr. Jiaping Lai, Nanking University, Tian Jin (China) (until 8/04)
Dr. Trevor Mathieson, NIWA, Auckland (New Zealand) (10/04 – 12/04)
Dr. Evgene Mikhailov, State University, Petersburg (Russia) (until 1/04)
Valeria Tékus, University Pècs, Hungary (2/04 – 6/04)
Dr. Minli Yang, University Peking (from 8/04)

Student Assistants

Ulf Dettmer (4/04 – 6/04)
Ferdinand Haller (4/04 – 6/04)
Abdel Salam Ikhlawi (until 4/04)
Thiam Bon Lim (5/04 – 7/04)
Tobias Roßteuscher (8/04)
Anna Todinova (7/04 – 9/04)
Diem-Hang Tran-Nguyen (6/04 – 9/04)
Dipl.-Biol. Iris Vomberg (until 3/04)
Samuel Wilberforce (7/04 – 8/04)