TECHNISCHE
UNIVERSITÄT
MÜNCHEN

Institute of Hydrochemistry

Chair for Hydrogeology, Hydrochemistry and Environmental Analytical Chemistry

Annual Report

2005

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,

the Year 2005 has seen a paradigm shift at universities in Germany. The years before were devoted to science more or less exclusively. Now, in times where government and most funding organisations show an empty money bag, education is more and more in focus of universities again. Impair partition of scientific skills between non-university institutions and university institutes will be the consequence in the long run.

2005 has seen an enormous increase in admitted student's number for chemistry, biochemistry, chemical engineering, and geological sciences. On the other hand total number of employees at the institute has touched a minimum of 40 for the first time. Only mobilisation of reserves allowed starting of 5 new PhD terms.

Germany presently lacks a regular budget (due to a change of the federal administration in November 2005) with the consequence that no new projects can be funded by the government. Hence, the institute has to pre-finance new projects on its own - with the hope to become reimbursed soon.

Besides these general restrictions we are in a phase of realignment. End of 2005 the anticipated completion of a S 1 microbiology lab became true. In parallel we are happy to welcome Dr. Seidel, who starts now with microarray developments for microorganism detection. Analysing the trend in Analytical Chemistry partitioning of the "market" into mass spectrometry, microfluidics/microarrays and bio-receptor based applications can be expected. Our contribution for future will be creation of microarray-based tools and generation of excellent antibodies.

Spectroscopy is still an important part of the house. After the successful launch of the photoacoustic soot sensor for diesel exhaust monitoring, we now try to develop particle separation schemes, based on the photophoresis effect. A new project with General Electric Europe deals with depth-resolved photoacoustic spectroscopy for optical tomography as early diagnostic instrumentation for breast cancer detection.

As can be seen, a lot of challenges are ahead of us. I like to thank this year especially the whole crew for their high performance. Two ongoing habilitation procedures demonstrate this. My very special congratulations go to Sebastian Wiesemann. He became a master craftsman (precision mechanics) this year, and will hopefully continue to support our research with his outstanding expertise. Günter Dollinger, the former head of our mechanical workshop, and Karin Koller, the well-versed financial accountant for many years, both retired. Thanks a lot for a wonderful cooperation!

I would also like to thank the various funding institutions, not to forget the "Freundeskreis" of the institute. A small circle of alumni and friends, but very needed now!

All the best for the year 2006

Reinhard Nießner
Head of the Institute

Head of the Institute and Group Leaders 2005

C. Haisch T. Baumann M. Seidel H. Prestel

R. Nießner M. Weller A. Held D. Knopp

1 Research

1.1 Hydrogeology and Hydrochemistry

1.1.1 Development and Protection of Ground Water and Mineral Water

Funding: Private Enterprises

Geothermal energy is considered a sustainable resource and the Federal Government offers high subsidies for the production of renewable energy. The jurassic sediments below the tertiary basin in Southern Bavaria are one of the primary targets for the exploration of deep geothermal energy. At least half a dozen groundwater wells reaching into the jurassic sediments have been built or are under construction in the close vicinity of Munich alone. They are offering a new look into the geological, hydrogeological, and hydrochemical settings of the Malm aquifer.

The Institute of Hydrochemistry is working together with state offices and private consulting firms to evaluate this data and to assess the long-term impact of geothermal energy production. The hydrochemical composition of the Malm aquifer is studied in a Diploma Thesis. This work will address the hydrostratigraphy and possible interactions with the sediments of the tertiary basin. The Thesis will also address possible hydrochemical effects of the reinjection of cold water into the Malm aquifer. It is well known from other places, that neglecting the hydrogeochemical equlibria will lead to serious problems affecting the long-term productivity of the groundwater wells.

Some of the deep groundwater wells are not only used for geothermal energy production, but also for providing water for balneo-therapeutical use, while others are driven into deep aquifers for balneological purposes alone. An assessment of the long-term effects of groundwater production from deep groundwater aquifers will be one of the high priority research targets. It is also necessary to think about possible treatment and reinjection techniques at sites with high volume withdrawal.

(*T. Baumann*)

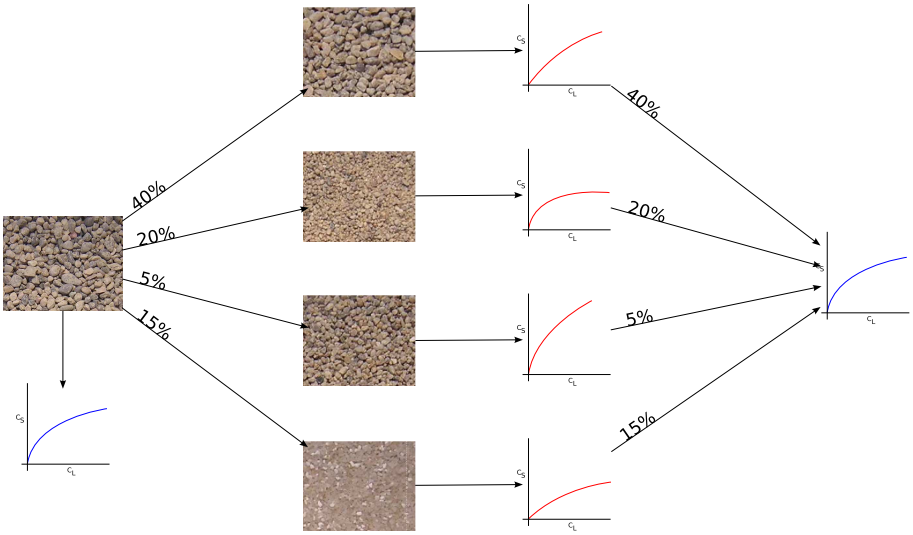
1.1.2 Development of a High-Throughput Test Design for the Determination of Sorption Parameters

Funding: IWC

Today groundwater is at risk of contamination by pesticides, herbicides, pharmaceuticals and fertilisers. To assess the transport properties of a contaminant in a specific soil, the matrix interactions have to be quantified. The proposed miniaturised sorption test uses existing microwell plate (MWP) technology to combine the most widely used sorption test methods (the conventional batch and column test), to estimate the sorption coefficient of a contaminant in sediment. The MWP has 96 wells, an integrated filter, is ready for high throughput analyses, and the calibration is performed

on-plate. Relative to a batch test with larger samples masses the heterogeneity of the sediment gives a larger variance of the sediment area between different wells. In the MWP sorption test, the sediment is therefore sieved in different fractions, which can either be placed on the same or separate plates. In this study the miniature batch test setting on the MWP was evaluated with experiments and simulations, so as to assess the reliability of this method. During this process a better way of sealing the MWP, a Quickfill method and a method of measuring the adsorption of nitrate have been developed.

A theoretical simulation was done to show how the fundamental sampling error increases when the sample mass gets smaller. It showed that a 95% confidence interval of the specific surface area of the sediment sample only increased 2-3 times when decreasing the mass from 10 g to 0.5 g per sample. To determine whether a potential mass error of the Quickfill method would have a magnified error propagation on the estimation of the sorption coefficient (K_d), a simulation using the concept of the Freundlich isotherm was done. The K_d-value inherited the mass error without magnification, and the n-value was about 3 times more robust.



Two MWP sorption tests of sulforhodamine-B (SRB) onto the same fraction of calcareous gravel gave reproducible sorption coefficients, with an overall analytical error of about 20% for both plates. Two different mineralogical fractions were tested together on the same MWP. Significantly different sorption was determined between calcareous gravel and thermal treated quartz, with almost the same size fraction. Simulations on the results from two MWP tests determined that the accuracy of the sorption test is decreasing from 100% to 80%, if 2 columns are used instead of 6 columns, while the uncertainty increases (95% confidence interval) from 40% to 80% of the mean K_d-value.

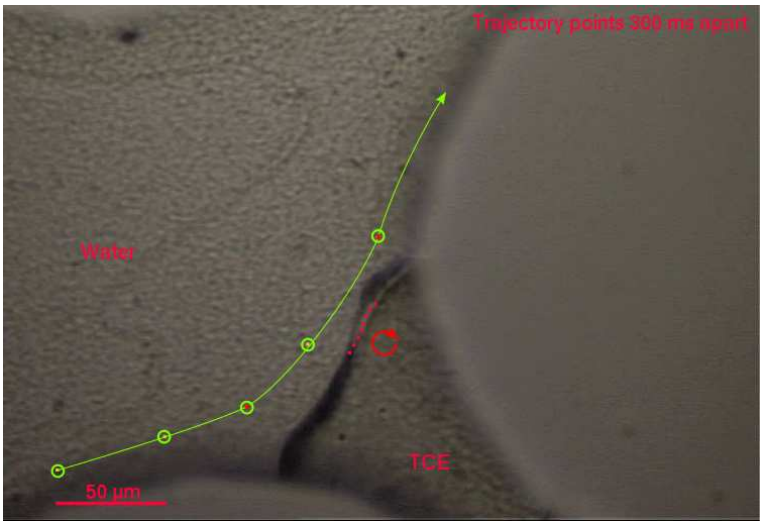
A method to measure sorption of nitrate on the MWP was developed. It uses UV absorption at 210 nm. A successful MWP test conducted on nitrate confirmed that there is no sorption of nitrate onto one fraction of calcareous gravel. Since nitrate has been assigned as a priority contaminant by the EU Environment Protection Agency, a miniaturised nitrate sorption test on the MWP is needed. The possibility of developing a nitrate test that uses a MWP plate reader looks promising.
(*C. Nilsson*)

1.1.3 Colloid Transport in Multiphase Systems

Funding: DFG Ba 1592/3-1

The mobility of colloids is partly controlled by filtration effects. In saturated porous media colloid/matrix interactions and dynamic properties are responsible for attachment and detachment processes. In the unsaturated zone, or if non-miscible fluids are present, the air/water interface and the water/fluid interface add to the complexity of the colloid transport phenomena.

The colloid processes at the interfaces in multiphase systems were examined on a single-particle level using micromodels. Four different sizes of fluorescent colloids were used in homogeneous and heterogeneous pore structures. n-Octanol was used as a non-miscible phase in the saturated experiments. Experiments in unsaturated micromodels were run at different ionic strengths and with varying pH-values. Experiments were run under flow and under no-flow (i.e. diffusion only) conditions.



Imaging results show that colloids are preferably captured at the various interfaces (air/water, air/water/matrix, water/octanol). Attachment to the water/matrix interface was less important. Dissolving gas bubbles caused a sudden release of colloids. Capillary effects influencing the mobility of colloids were observed under unsaturated conditions. The attachment to the water/octanol interface depends on the surface functional groups of the colloids. The quantification of these processes is in progress.
(*T. Baumann*)

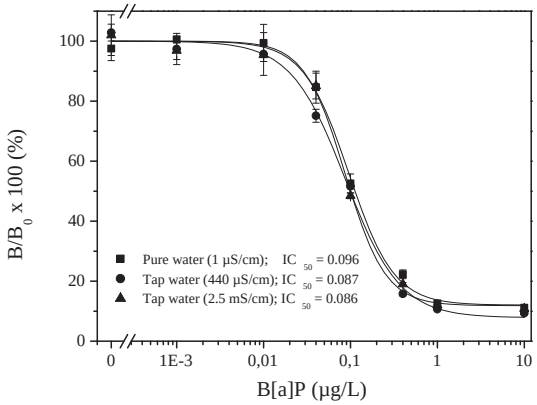
1.2 Bioanalytics I

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

Funding: BMBF 02WU0290

Because of their carcinogenicity and spreading in the environment polycyclic aromatic hydrocarbons (PAHs) have caused increasing attention in recent years. In Europe, a threshold limit of 10 ng/L was set for benzo[a]pyrene (B[a]P) in water intended for human consumption (Council Directive 98/83/EC) and, therefore, sensitive and reliable methods are needed to evaluate its presence. We report here on the development of a highly sensitive indirect competitive ELISA for the detection of B[a]P in tap water.

Fourteen monoclonal antibodies were generated in mice using novel B[a]P derivatives. The ELISA with the least interference and the best sensitivity was optimized and characterized. As co-solvent, ten percent of methanol (v/v) were optimal. With the purified antibody (22F12) the average IC_{50} for B[a]P and corresponding detection limit at $S/N = 3$ was 65 ng/L and 24 ng/L, respectively. From the 16 EPA PAHs, only chrysene, indeno[1,2,3-cd]pyrene, and benzo[b]fluoranthene showed a cross-reactivity (CR) higher than 20%. No CR was observed for two- and three-ring PAHs as well as dibenz[ah]anthracene and benzo[ghi]perylene. As possible matrix interferences the effect of pH value (range 6.9 - 9.5), ionic strength (specific electric conductivity 1 μS/cm - 2.5 mS/cm), and inorganic ions (sodium, copper, iron, aluminium, manganese, chloride, sulfate, nitrate, and nitrite at maximum permissible levels according to the Council Directive) on both signal and sensitivity of the ELISA was studied. No significant influence of these parameters on the ELISA competition curve was found. We suggest that the optimized ELISA can be used to monitor tap water samples without extraction and cleanup at B[a]P levels close to the limit value of the new drinking water directive.



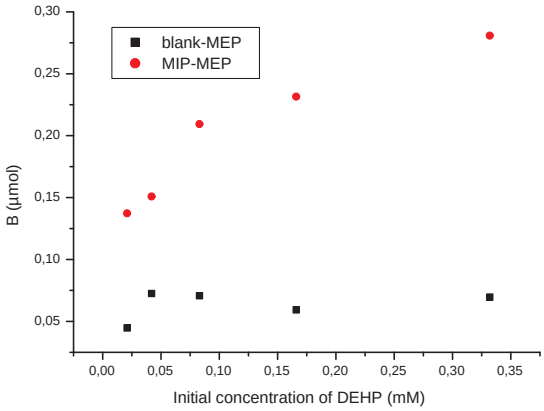
ELISA competition curves for B[a]P prepared in water of various ionic strengths with the best monoclonal antibody generated in this project are depicted in the figure. (*D. Matschulat, A. Deng*)

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

Funding: EU QLK-4-CT2002-02323

The subproject focuses 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.

In this period, much emphasis of research work was devoted to decrease the size of sub-micron particles on order to allow easier coating of sensor surfaces. To achieve this, two different methods, precipitation polymerization (PP) and mini-emulsion polymerization (MEP) were used. To compare the affinity of the different particles, rebinding experiments were carried out in different solvents. MIPs prepared by both methods clearly showed the imprinting effect in pure acetonitrile. However, the polymer which was prepared by MEP exhibited a significant higher rebinding capacity (see Figure).



Further, polymer particles (32 - 63 μm) which were obtained by bulk polymerization were packed into stainless steel HPLC columns to estimate the retention behaviour of nineteen different EDCs on DEHP-MIP column and corresponding blank polymer. The capacity factors and imprinting factors were calculated.

Finally, a validation experiment was performed with unknown spiked pure water and filtrated surface water samples (single compound solutions and mixtures containing up to 3 analytes).

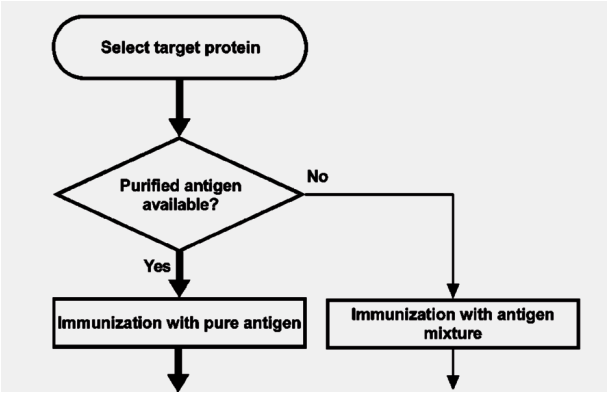
(*M. Yang*)

1.3 Bioanalytics II

1.3.1 Screening Methods for the Efficient Development of Sandwich Immunoassays

Funding: EU QLRT-2000-01151
Cooperation: FA 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)

In the project "AllergenTest", funded by the EU, we examined different methods to screen for suitable antibody pairs. A practical problem is caused by assays, which are based on two monoclonal antibodies of the same species, in most cases from mouse. Conventional detection methods with secondary antibodies targeted against mouse immunoglobulins are not applicable. One of the antibodies would have to be labeled, which however, would require that this antibody is available in sufficient amounts and in a purified form. Both conditions are not met in an early stage of antibody screening, when the decisive selection step has to be done. We tested the direct biotinylation of unpurified cell supernatant, enzyme-labeled polyclonal antibodies, enzyme-labeled Fab fragments, enzyme labeled protein G, and as a reference method the direct covalent labeling of antibodies (peroxidase). It could be shown that most of the methods do not show sufficient signal to background levels to be useful in practice. Particularly the methods based on anti-species antibodies or antibody fragments can be recommended. Furthermore, it could be shown that the affinity constant of the antibody/antigen complex plays a dominant role in the clone screening process. Microplate-based methods are particularly fast, which is necessary under the time-pressure of clone-screening projects. Finally, we proposed a novel strategy for the efficient identification of matching pairs. Important points are the selection of the target antigen (immunization with mixtures should be avoided in nearly all cases), and the affinity screening. Here we propose to use the antibody of the highest affinity to use as a detection antibody, although later in the final test, this antibody should be used as capture antibody. The reason for this paradox recommendation is the fact that the antibody concentration can be easily normalized by using a precoating with anti-mouse antibodies, and hence, not even the concentration of the antibodies to be screened has to be known.

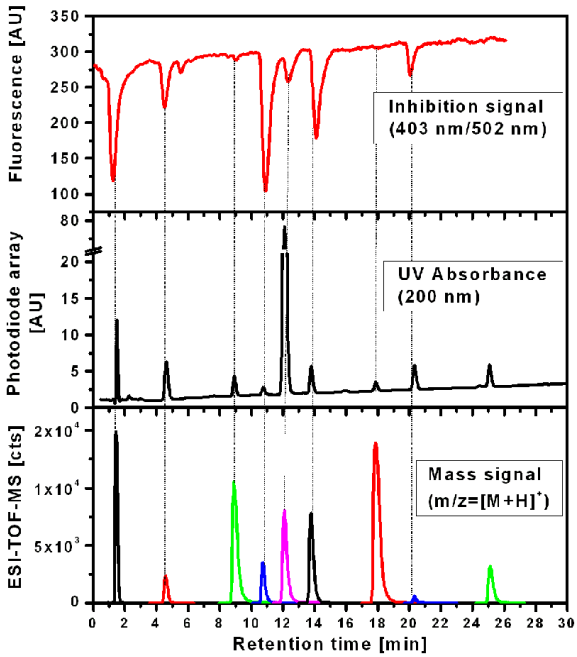


The final workshop of the project "AllergenTest" was held on May 18, 2005, in Tulln, Austria. Additional information can be found on the project website.
(*M. G. Weller, M. Kiening*)

1.3.2 Effect-Directed Analysis of Toxins by LC-MS Hyphenated With Enzyme Inhibition Detection

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

The purpose of effect-directed analysis is the direct connection of instrumental analysis and toxicity test. This is necessary, because nowadays the progress in instrumental analysis at the trace and ultra trace levels oversaturates the public interest with a data flood of irrelevant substance concentrations. Therefore and also in terms of cost saving, it is reasonable to concentrate on the analysis of toxic relevant compounds in suspected contaminated samples. However, the determination of unknown toxicants by HPLC separation is tedious due to missing standard substances. The monitoring of toxic effects in environmental samples by toxicity tests with living organisms is only of limited relevance, as simply acute toxicity is detected and the molecular cause of toxicity is often only vaguely indicated. The combination of toxicity test at the molecular level with a physical-chemical separation step allows the development of a rapid and cost-efficient detection method for the demand of effective environmental analysis.



For the effect-directed analysis of toxins a hyphenated system was designed, which links a high performance liquid chromatography device with photodiode array and mass detector to a continuous biochemical detector. To build a model system for a neurotoxicity-directed analysis the activity of the enzyme acetylcholine esterase is monitored with the biochemical detection unit. A sample (water with spiked insecticide standards) is separated with reversed phase chromatography on a C18 column. The column outlet is split into three flow paths. The first flow path leads the eluting analytes to a photo diode array to measure the absorbance depending on the wavelength. In the second flow path the analytes enter an electrospray ionization time-of-flight mass spectrometer for the confirmation of the molecular mass or structural identification by optional fragmentation. In the third flow path the analytes flow into an online enzyme inhibition assay. The residual enzyme activity is measured homogeneously and continuously by monitoring the conversion of the substrate acetoxy-methyl-quinolinium iodide by fluorescence measurement. A negative signal peak caused by reduction of enzyme activity indicates the elution of potentially toxic compounds. To overcome severe band-broadening in the slow post-column reaction system due to parabolic flow profile, gas segments were introduced at a high frequency. The chromatograms of a spiked water sample (several insecticides) show largely the same resolution for the enzyme inhibition detector signal with a reaction time of ten minutes compared with the resolution of the immediately measured mass and absorbance signal (see figure).
(*S. Fabel*)

1.3.3 Development of an Automated Microarray System for the Detection of Antibiotics in Honey

Funding: Eurofins, Hamburg

Honey is considered to be an extremely complex matrix for analysis. This is true for conventional techniques, as well as for bioanalytical methods, such as immunoassays or biosensors. Honey can be contaminated by antibiotics on different routes. In Germany, antibiotics such as streptomycin are used for the control of the bacterial plant disease "fire blight". In addition, increasing amounts of honey are imported from nearly all continents. This leads to the situation that even antibiotics, which are banned in Europe, can be found in honey samples. The conventional quality control of honey is an expensive and lengthy process. Therefore, fast screening methods for honey are highly desirable. In this feasibility study, the Parallel Affinity Sensor Array (PASA) system, which had been developed for the ultrafast detection of antibiotics in milk, was applied to honey samples of different origin. The sensor system was switched to a regeneration mode, since other studies have shown the significant advantages of this approach. Monoclonal antibodies against erythromycin, sulfamethazine, tylosin, streptomycin, neomycin, tetracycline and chloramphenicol were tested. For reference purposes a trinitrotoluene antibody was used.

Regenerations were achieved over more than 20 cycles, which means that the costs per analysis would be much lower than in systems with disposable chips. Assay sensitivity is adequate in the case of erythromycin, sulfamethazine and tylosin, and the legal limit of streptomycin might be reached after some minor optimization. For neomycin and chloramphenicol, better antibodies are needed. Particularly chloramphenicol is a difficult case, since the limit is 100 times lower than for the other antibiotics mentioned. In this project, matrix effects have been studied, also. It could be shown that standard blocking approaches are not efficient to reduce these interferences. Probably, they are due to some true cross-reactions or unrecognized contamination by antibiotics. In this project, the parallel detection of antibiotics in real honey samples was achieved in a relevant concentration range. Hence, microarray biosensors seem to be a powerful tool for the quality control of honey.

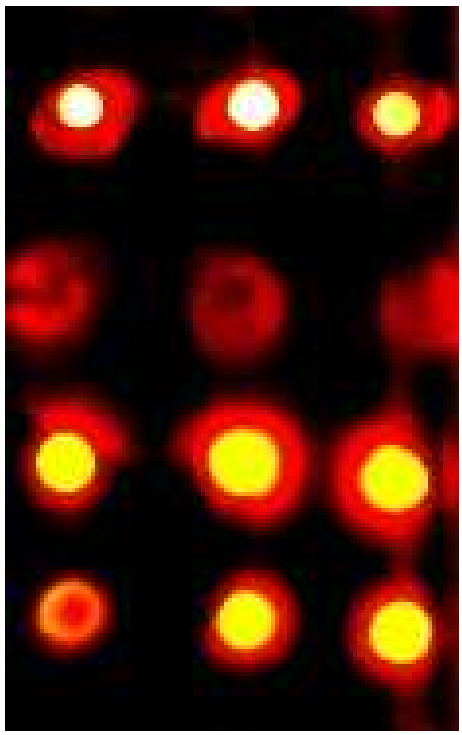
(*B. Knecht, M. G. Weller*)

1.3.4 Development of Hapten Microarrays for the Detection of Antibiotics in Milk

Funding: IWC

In the past few years a parallel affinity array (PASA) for the rapid automated analysis of a broad spectrum of antibiotics in milk has been developed at the Institute of Hydrochemistry using multianalyte immunoassays with an indirect competitive ELISA format. Herein protein conjugates carrying haptens are immobilised as tiny spots on modified glass surfaces.

Based on this sensor system, a new kind of microarray was developed, where activated haptens are bound to a modified glass substrate via polyethylene glycol (PEG) diamine linkers. In addition to the homobisfunctional PEGs, heterobisfunctional methoxy PEG amines were used for surface coverage. This PEG surface was intended to resist nonspecific binding of proteins. Another motivation to create such a chip was to achieve a more distinct way the antibiotics are presented on the surface. In addition, this kind of surface was expected to possess a higher durability and to show a better regenerability for continuous use than chips based on conventional surface chemistry.



To create such a hapten array, the surface of a glass substrate was first activated with epoxy groups through silanisation with 3-glycidyloxypropyl trimethoxysilane. Then homobisfunctional PEG diamines (MW ca. 2 kDa, 3 kDa or 10 kDa) as well as heterobisfunctional methoxy PEG amines (MPEGs, MW ca. 2 kDa) were attached to the modified glass surface in varying molar mixing ratios (MPEG/PEG diamine 100:1 to 500:1) and different combinations of chain lengths. For covalent attachment, epoxy derivatives of the antibiotics sulfamethazine (SMA), sulfadiazine (SDA) and streptomycin were synthesized by reaction with a bisoxirane.

Regeneration cycles were performed by using a HCl/glycine buffer containing 0.1% of sodium dodecyl sulfate. After 46 regeneration cycles the signal intensities of streptomycin, SMA and SDA still showed 38%, 48% and 50% of the initial values. By the use a regenerable chip, standard calibration curves of all three antibiotics were measured in milk. For streptomycin a test mid-point of 5.9 μg/l and an optimum test range of 1.0 - 32 μg/l, for SMA a test mid-point of 11.4 μg/l and an optimum test range of 1.7 - 68 μg/l and for SDA a test mid-point of 15.7 μg/l and an optimum test range of 2.1 - 105 μg/l was achieved. Due to the rather low detection limits, this microarray should be applicable for the control of streptomycine, sulfamethazine and sulfadiazine residues in milk.

(*A. Wolter*)

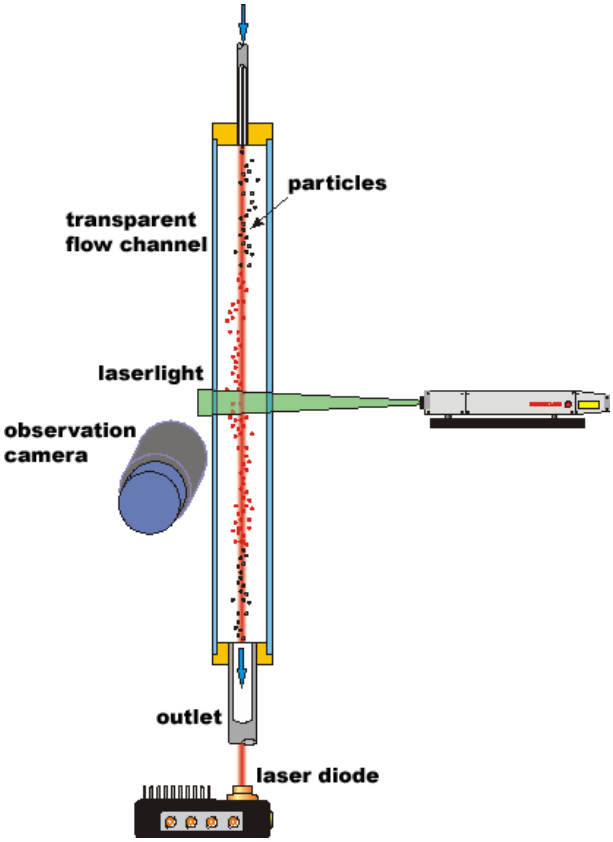
1.4 Applied Laser Spectroscopy

1.4.1 Photophoretic Particle Separation

Funding: DFG Ni 261/16-1

Photophoresis denotes the phenomenon that very small particles suspended in gas or liquid are moving when they are illuminated by a sufficiently intense beam of light. Motion can occur in the direction of light (positive) and against that direction (negative). In conventional separation techniques aerosols and colloids are separated by means of electrical, thermal or flow fields. Funded by the DFG, the application of light is tested as a possibility of separating particles due to their optical properties. Such a separation technique would allow e.g. the isolation of organic from inorganic particles of the same size.

We aim to develop a continuous flow separation system for aerosols regarding the optical properties of the particles. Hence, we started with a first setup to characterize the thermo-photophoretic effect by using particles of different size and absorption coefficients. The system basically consists of a silica capillary positioned vertically at normal pressure conditions with the inlet on top and an outlet at the bottom.



The particles inside the capillary move downwards forced by an air flow stream or by gravity. A diode laser under the capillary is used to levitate the particles by means of photophoretic force. The process can be observed by an single lense reflex camera. For quantitative measurements, we use a vibrating orifice aerosol generator to produce monodisperse particles and a condensation nucleus counter for detection. The results from the setup will help us to design a suitable separation system.

Better knowledge of the optical properties of different aerosols leads to a better understanding of our climate system and its changes that can occur due to variation of aerosol concentrations in the atmosphere.

The photophoretic force acting on particles suspended in water is generated by a homemade diode laser. The laser provides an optical power of up to 2 W at a wavelength of 808 nm out of an optical fibre to drive various optical configurations. In order to sort the particles due to their optical properties, several configurations are proposed. The laser light can be directed either in or perpendicular to the direction of flow. In any case, the particles are observed in orthogonal direction by a microscope at a magnification of 20. A CCD-camera on top of the microscope is connected to a personal computer and records the movement of the particles. The extraction of the trajectories from the images is performed by proper analysis of the recorded images. A special routine for calculating the photophoretic velocity was established for image processing software. In first basic experiments on transparent latex particles suspended in water, the photophoretically induced motion could be shown in the absence of any thermal disturbance.

The main focus of this work lies on the optical configurations in order to optimise the interaction between particles and light to achieve high separation yields.

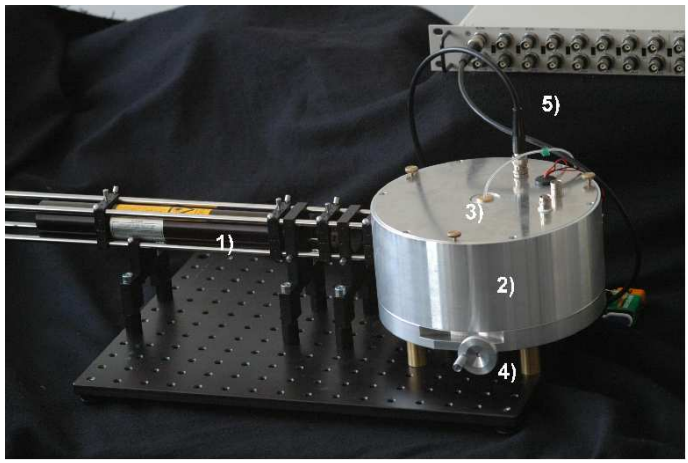
(*C. Kykal, C. Helmbrecht, C. Haisch*)

1.4.2 Light Scattering for Hydrocolloid Detection

Funding: IWC
Cooperation: Stadtwerke München

In case of a sudden rise of the ground water level, combined with heavy rainfall, surface water may directly connect to groundwater. In those cases groundwater wells are at risk of microbial contaminations. To maintain the safety of drinking water, a fast and selective detector for microbial contaminations is required. The sensor will trigger an immediate shutdown of the contaminated wells, thus reducing the risk of a contamination of the storage tanks and distribution systems.

Detection of the bacteria will be carried out by a combination of light scattering and fluorescence. Light scattering allows determining particle number and size. Bacteria are larger than most other particles contained in ground water (>1μm). The beam of a HeNe-laser ($\lambda = 633\,\mathrm{nm}$) illuminates the water flow in a capillary and the radiation scattered by the particles is detected by means of several photodiodes. To assess the most significant detection angles, the photodiodes are scanning along a semicircle around the capillary. The voltage of the photodiode measured at a respective angle is read out by a computer. By the help of Mie theory, the measured voltage distribution reveals the size distribution of the particles.

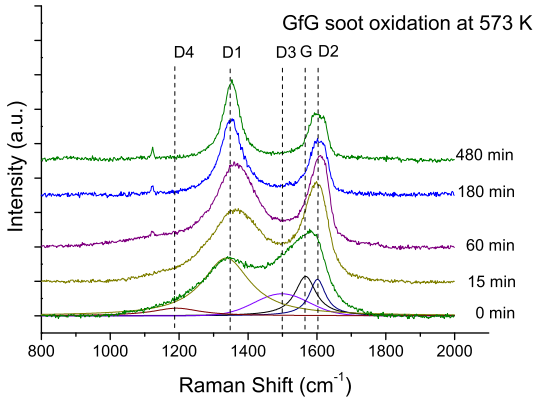


All living cells possess an amino acid, Tryptophan, which has a strong fluorescence with a maximum at $\lambda = 353\,\mathrm{nm}$. If the detected particles are bacteria, fluorescence of this amino acid can be observed. For the stimulation of the fluorescence a further light source with a wavelength maximum at 280 nm will be applied. In a right angle to this excitation light source, a photomultiplier is arranged which detects the fluorescence light. Selection of the fluorescence emission wavelength range will be done by means of a bandpath filter in front of the photomultiplier tube.
(*S. Jähme, C. Haisch*)

1.4.3 Raman Microspectroscopic Analysis of Changes in the Structure and Reactivity of Soot Undergoing Oxidation and Gasification

Funding: IWC

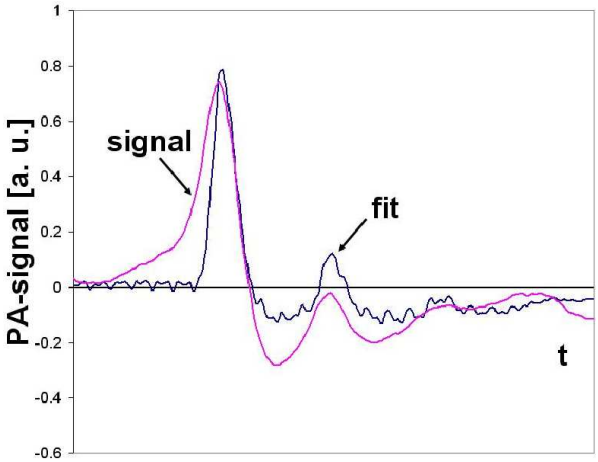
Raman spectroscopy is based on the effect of inelastic light scattering due to changes in the polarizability of the electron cloud in molecule and associated with measuring of molecular vibrations. Raman spectroscopy provides “fingerprint” spectra that are unique to each specific compound and contain information about chemical composition and structure. It requires no or little sample preparation (direct measurements can be carried out on solids), and Raman spectra can be obtained non-invasively. Moreover, the coupling of Raman spectroscopy with microscopy (Raman microspectroscopy) enables high spatial resolution and sensitivity (laser beam diameters as small as 1 μm).



Raman microspectroscopy has been applied to follow structural changes in spark discharge (GfG) and light duty diesel vehicle (LDV) soot upon oxidation and gasification by nitrogen oxides and oxygen at 523 and 573 K. Raman spectra have been recorded before and in the course of the oxidation process, and spectral parameters have been determined by curve fitting with five bands (four Lorentzian bands (G, D1, D2, D4) and one Gaussian band (D3)). For GfG soot a steep decrease of the relative intensity of the D3 band is found to indicate rapid preferential oxidation of the amorphous/organic carbon fraction, and a decrease of band widths (full width at half maximum, FWHM) indicates an increase of structural order of the graphitic carbon fraction and decrease of chemical heterogeneity in soot. The spectroscopic changes are in agreement with a strong decrease of chemical reactivity (rate coefficients of oxidation and gasification) as the mass conversion ($\eta_m = 1 - (m/m_0)$, where m_0 = initial mass and m = residual mass) of GfG soot increased. In contrast, the spectral parameters and reactivity of LDV soot remain largely unchanged. Overall, the spectroscopic and kinetic findings suggest that Raman spectroscopic parameters – in particular the D1 band width and the D3 band intensity – characterize the relative abundance and structural order of the graphitic and amorphous/organic carbon fractions, respectively, and can be used as proxies for the chemical reactivity of soot.
(*N. Ivleva*)

1.4.4 Biofilm Observation with Confocal Laser Scan Microscopy and Photoacoustic Spectroscopy

Funding: DFG Ni 261/14-2



Biofilm is an agglomeration of bacterial cells embedded in a matrix of extracellular polymeric substances, built by the bacteria themselves. It is formed at aqueous interfaces and is a major problem for heat transfer and current flow in water-exposed systems, causing high costs. Monitoring of biofilm growth helps to optimize backwashing and biocide dosing, thus saving industry lots of money.

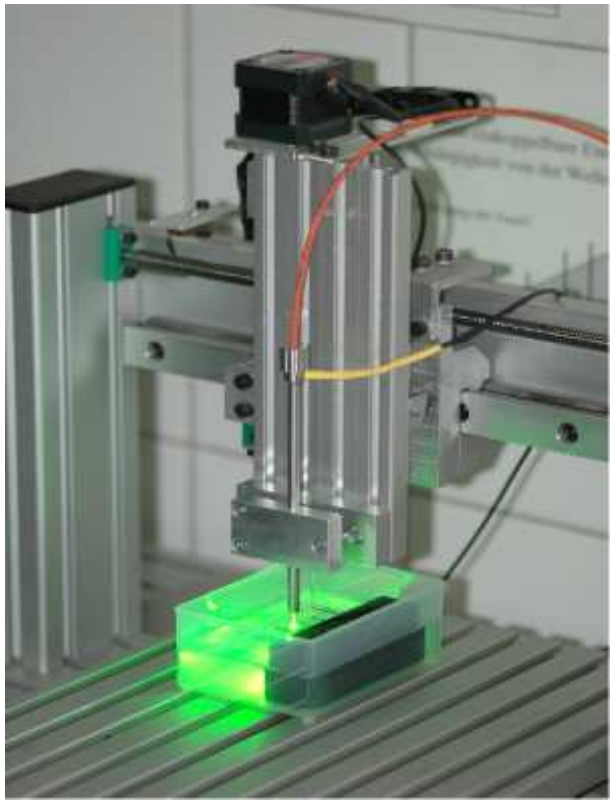
A monitoring system based on photoacoustic spectroscopy (PAS) has been established at the IWC, and a characterization of its ability for biofilm monitoring has been conducted. Several experiments regarding biofilm growth, structure and removal showed its applicability for online and in-situ biofilm monitoring. Being a new method in biofilm observation, results obtained with photoacoustic spectroscopy have to be verified. This is done with a standard method for biofilm observation, confocal laser scan microscopy (CLSM), as reference method. For comparison of results, depth-resolved experiments are conducted. In CLSM, substratum coverage in every layer of a stack is examined. Using statistical determination of 20 positions on a biofilm grown on glass objective slides, average substratum coverage, depending on depth of the sample, was obtained

In PAS, thin films were used as reference samples for depth-resolved signals of the absorption coefficient. Reference samples were prepared using spin-coating and scraping. Signals of those are regarded as "Basic Signal Units" (BSUs) for signals of unknown samples. A deconvolution algorithm, taking into account sample depth z and loss of initial energy through absorption according to Lambert-Beer law, is outlined.
(*C. Haisch, T. Rossteuscher*)

1.4.5 Analysis of Optical Inhomogenities in Aqueous Media with a Focussing Photoacoustical Sensor Probe

Funding: IWC

The analysis of optical inhomogenities in highly scattering aqueous media is fundamental to various fields of interest. Photoacoustic (PA) spectroscopy is versatile technique meeting this requirement. PA is a combination of photonics and acoustic sound waves, which are generated local light absorption and, in consequence, local warming and expansion in the sample. In contrast to other imaging techniques, light scattering does not affect the image quality as long as light can penetrate deeply enough.



While the main focus of PA application at the IWC of the past few years was a 1-dimensional approach to the investigation of layered structures such as biofilms and other depositions, the high directivity of the developed sensor probe allows the reconstruction of 3-dimensional absorption distributions by lateral scanning of the probe.

Following a constant improvement of the sensor probe design, we pursue the aim to determine the imaging parameters depth resolution, lateral resolution, detector directivity and sensitivity, pushing forward the limits of detection. By light field investigations (Monte-Carlo simulation) and the scanning of artificial light-absorbing structures, we are able to provide a full characterization of our imaging tool.

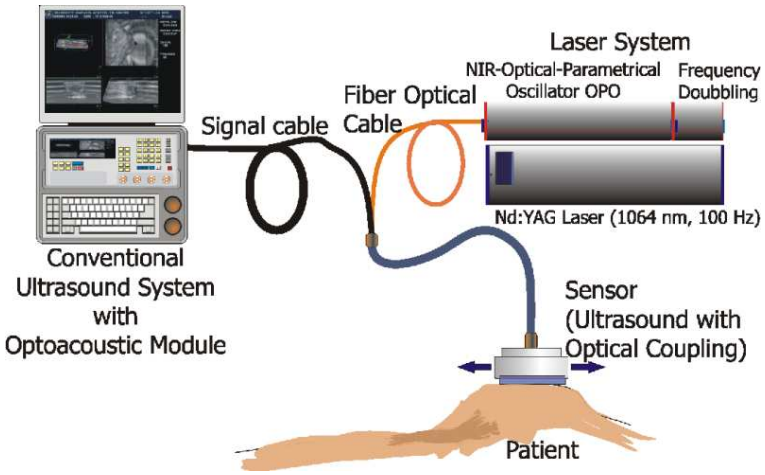
Major applications are the diagnostics of human tissue for metabolism studies and cancer detection and the absorption analysis of all kinds of scattering chemical structures.
(*L. Hofmann, C. Haisch*)

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

Funding: Bayerisches Staatsministerium für Wirtschaft, Infrastruktur, Verkehr und Technologie, Program: BayMed
Cooperation: General Electrics, München; InnoLas, München

Depth-resolved Photoacoustic (PA) spectroscopy of solids and liquids has been and is still applied for a variety of analytical tasks ranging from biofilm monitoring to non-invasive blood glucose determination. The OPUS project again is a PA approach to a medical problem.

The most common method for breast cancer detection nowadays is the mammogram. Drawbacks of this technique are the application of potentially harmful, ionizing radiation and, under certain conditions, a limited contrast. An alternative is conventional sonography, which, again, is hampered by low contrast due to the very limited variations of the acoustical properties of healthy and cancerous tissues. Laser excitation of the PA effect in combination with the imaging qualities of a conventional ultrasound detector can offer additional information, e.g. about locally increased blood circulation, oxygen consumption or even angiogenesis, which may be indicators for malignant tumors.



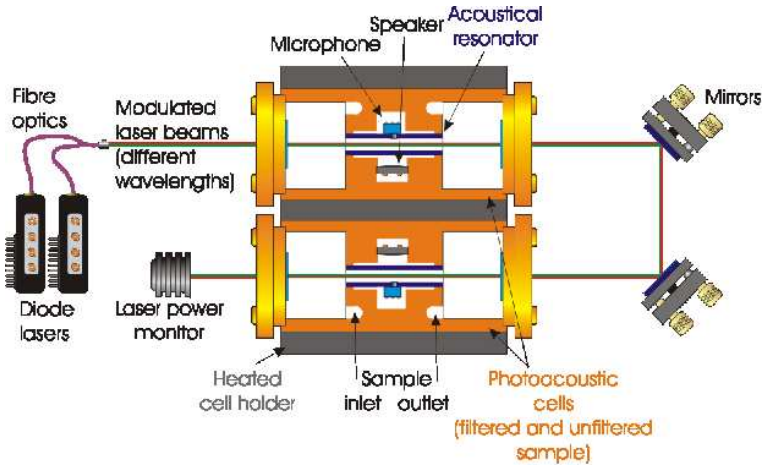
For routine application of such system, a high-repetition rate, pulsed, wavelength-tunable laser is required, which is about to set-up at the cooperation partner InnoLas. At the IWC, optical and optoacoustical properties of human tissue are collected from literature and measured, resp., in order to fully understand sound generation and hence, to optimize image deconvolution. Tissue phantoms will be fabricated to test the system's performance. Furthermore, IWC is in this project responsible for the selection of relevant wavelengths and for the adaptation of the optoacoustical system on the ultrasound sensor.
(*K. Zell, C. Haisch*)

1.4.7 Photoacoustic Characterization of Aerosol Optical Properties

Funding: DWD

Fine particles suspended in air, i.e. aerosol particles, play a major role for the earth's radiation balance. Forward and backward light scattering as well as optical absorption separately have to be taken into account for concise calculations. Up to now, the optical properties of aerosol in the lowest atmospheric layer (0 - 1000 m), has been widely neglected or roughly estimated.

Following a proposal of Germany's National Meteorological Service (Deutscher Wetterdienst) we develop and construct an instrument based on Photoacoustic (PA) Spectroscopy to measure optical absorption of particulate matter at different wavelengths. The system consists of two parallel, identical PA measurement cells. The core of these cells is a longitudinal acoustical resonator, containing the microphone detecting the optically induced sound wave. The modulated laser beam passes through the centre of the resonator tube, where it is absorbed by the aerosol particles. The deposed optical energy it converted into thermal energy, which leads to a modulated expansion of the gas atmosphere, i.e. a sound wave. The measured aerosol is sucked through the two cells, one directly and one after particle filtration. The difference of the two measured signals represents the particle's optical absorption. Due to the PA principle, light scattering does not contribute to the signal.



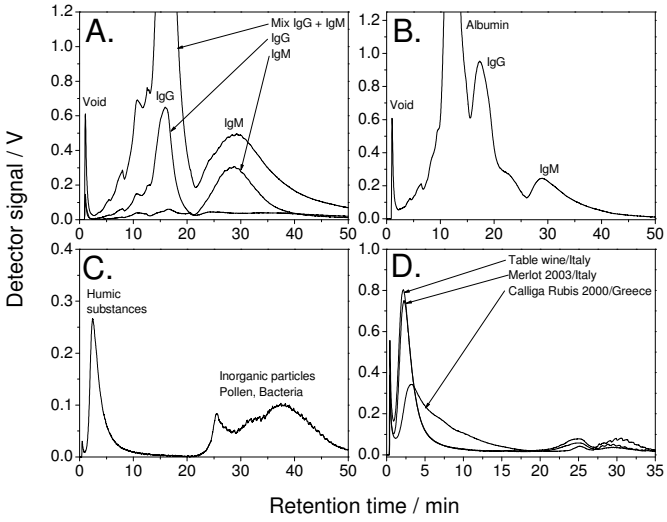
The system will be integrated into a small robust housing and will be completely computer controlled, allowing an automated, unattended operation over several weeks. The construction considers the fact that maintenance has to be carried out by personal not familiar with the details of the instrument and without special equipment.
(*C. Haisch*)

1.5 Nanoparticle Research

1.5.1 Characterization of Hydrocolloids Using Slot Outlet-Asymmetrical Flow Field-flow Fractionation (SO-AF^4) – New Applications

Funding: DFG Pa716/4-2

The goal of this project is the characterization of hydrocolloids, especially in municipal and industrial waste water treatment plants, and the investigation of their interactions with biofilms in laboratory reactors and technical plants. An asymmetrical flow field-flow fractionation (AF^4) system with slot outlet technique (SO) for in-channel enrichment of hydrocolloids was used for the characterization of artificial and natural hydrocolloids. This technique 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 hydrocolloidal systems, the AF^4 system can be coupled with online inductively-coupled plasma mass spectrometry (ICP-MS). The principle of sample enrichment is based on that the carrier is split into a colloid-free part and a sub-stream with increased colloid concentration. Different polymer standards, proteins, and self-synthesized tracer colloids, as well as real samples were used to assess the performance of the new technique. It enables signal improvement factors up to 14 and shows various advantages over enrichment methods, which already exist. Several new applications were developed, e.g. the separation of proteins, especially immunoglobulin G and M in antisera (see figure A: Immunoglobulin standards, and B: Rabbit 2,4-D antiserum), the characterization of hydrocolloids in liquid manure (figure C), and in wine samples (figure D).



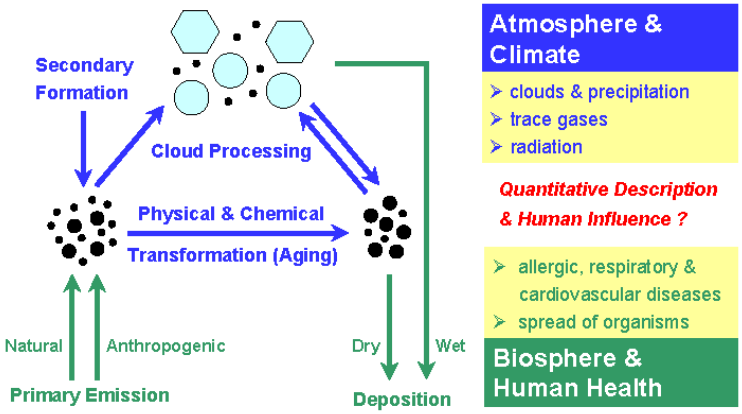
Additionally, larger amounts of monodisperse thulium(III)phosphate tracer colloids were synthesized for tracer experiments in biofilm reactors and, in the near future, a wastewater treatment plant. The results of the biofilm reactor experiments show a fast incorporation of the particles in the biofilm without influencing the degradation rate.

(*H. Prestel*)

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

Funding: BMBF (AFO2000, 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 $PM_{2.5}$); 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.

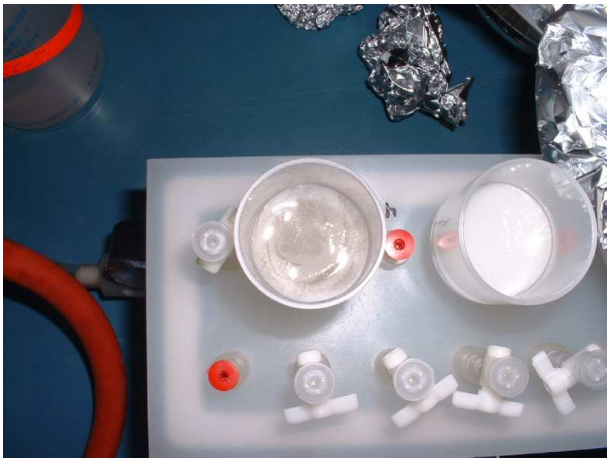
- Experimental investigation and mathematical modelling of the interaction of water vapor with aerosol particles of complex chemical composition (mixtures of salts and biopolymers, etc.): electric charge effects and microstructural rearrangements; phase transitions and hygroscopic growth; kinetic limitation 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, E. Mikhailov, U. McKeon, U. Pöschl*)

1.5.3 Detection of Microorganisms in Atmospheric Aerosol Samples by ATP Bioluminescence Reaction

Funding: IWC

A considerable fraction of the atmospheric aerosol is of biological origin. At present, the composition of these primary biogenic aerosol particles (dominated by parts and products of microorganisms as well as vegetation) is largely unknown. Obviously, essential organophosphorus compounds such as nucleotides, phospholipides and phosphorylated proteins are present in bacteria, fungal spores, pollen, algae, etc. Adenosine triphosphate (ATP) is the key molecule with regard to energy transfer and energy storage in all living cells. Therefore, this work is focused on the identification and quantification of ATP in atmospheric aerosol particles as a characteristic marker substance for living matter.



ATP is reliably detected by bioluminescence in a luciferase/luciferin system. After formation of a luciferase-luciferin-AMP complex, oxidation by O_2 leads to degradation of this complex and emission of light. Under controlled conditions, the photon emission is proportional to the sampled ATP concentration. Recently, the bioluminescence method has been applied for the identification of individual bacterial cells.

In this project, atmospheric aerosol particles were sampled on polycarbonate filters and incubated with tryptic soy broth. After enzymatic cell disruption the bioluminescence reaction was initiated by adding the enzyme solution. In order to improve the photon yield of the system, an ATP recycling step was introduced by addition of phosphoenolpyruvate and pyruvate kinase. The bioluminescence reaction is established and measured directly on the particle sampling filters. This allows for spatially resolved detection of ATP on the filter surface in future experiments.

Analyses of ATP standard solutions and atmospheric samples showed promising results for the application of this method to atmospheric aerosol particles. Further development ist needed to elucidate the influence of the sample matrix and different cell disruption methods, and also to optimize the enzyme system for better detection limits.

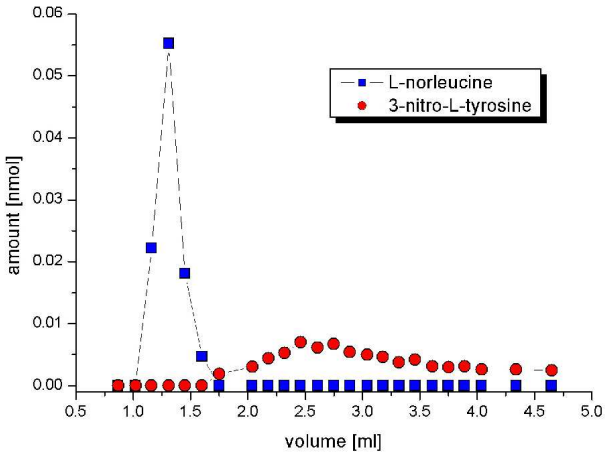
This work sets the basis for a reliable ATP detection method in the atmospheric aerosol which will ultimately lead to a better knowledge of the chemical composition of the organic aerosol fraction and a better understanding of the biogeochemical phosphorus cycle.
(*U. McKeon, A. Held*)

1.5.4 Determination of Proteins and Nitroproteins in Air Particulate Matter

Funding: BMBF (AFO2000, 7ATC05)

The chemical composition of fine air particulate matter ($PM_{2.5}$) is of high diversity and variability depending on sampling location and time. Biopolymers, e.g. proteins, are considered to make up 20 to 60% of the water-soluble organic carbon fraction. Proteins play a major role as airborne allergens and may undergo nitration when exposed to NO_2 and O_3 in atmospherically relevant concentrations. This posttranslational modification is likely to trigger immune responses and provides an explanation for the observed increase in respiratory diseases like asthma and allergies and its association to traffic-related air-pollutants like NO_2 and O_3.

In this work, two analytical methods were established for the detection of 3-nitrotyrosine in $PM_{2.5}$ and road/window dust samples: RP-C18-HPLC separation coupled to fluorescence detection and GC-MS analysis via negative chemical ionization. Due to matrix interferences a selective sample preparation step is needed after protein hydrolysis For this task, application of an anion exchange resin for selective enrichment of 3-nitrotyrosine in extract and protein hydrolysates of particulate matter was evaluated. Furthermore, immunaffinity chromatography utilizing anti-nitrotyrosine specific polyclonal antibodies was established (see Figure).



The protein content of aqueous extracts and macromolecular fractions (> 5 kDa) of $PM_{2.5}$ samples was determined by two protein quantification assays. The results were compared to and evaluated by amino acid analysis. Here, samples were derivatized and hydrolysed before separation by reversed phase high performance liquid chromatography.

Compared to amino acid analysis the microBCA assay overestimates the protein content in the macromolecular fraction by a factor of approximately 30, while the protein content determined by the NanoOrange assay is in the same order of magnitude as the protein content determined by amino acid analysis.

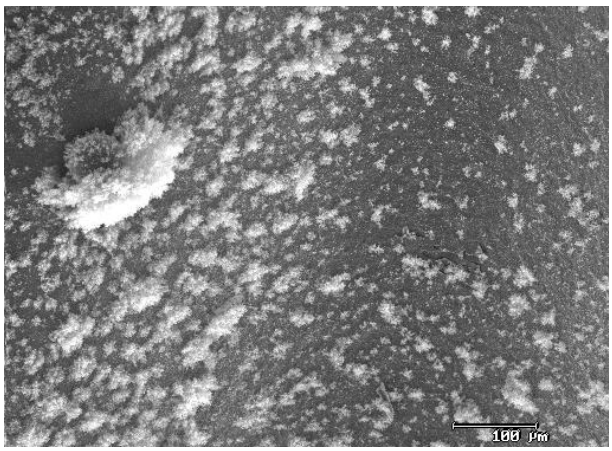
In the investigated samples from Hohenpeißenberg and Großhadern the protein fraction of $PM_{2.5}$ is less than 1%! Also, this study clearly showed that the conventional microBCA assay is less selective than the NanoOrange assay with regard to protein quantification.
(*T. Fehrenbach*)

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

Funding: Bavarian Research Foundation
Cooperation: MAN Nutzfahrzeuge AG, Nürnberg; Oberland-Mangold GmbH, Eschenlohe; Fritz-Haber-Institute, 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 focused 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 different 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 steelstructures 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 significant 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.
(*A. Messerer, D. Rothe*)

1.6 Microbiology & Microarrays

Funding: IWC
Cooperation: Stadtwerke München

At the end of 2005 a new field of research was opened at the IWC. The research group *Microbiology and Microarrays* has the objective to detect pathogenic and non-pathogenic microorganisms with modern bioanalytic methods quantitatively.

To reach these objectives a microbiological lab was built in the technical hall. The laboratory has the most modern equipment to use microorganisms under aseptic conditions. The lab is equipped, in addition, with an air-conditioning, which is important especially for the microarray production.

The topic of the research is the rapid but selective enrichment and the parallel detection of microorganisms. That's why the crossflow microfiltration and the immunomagnetic microfiltration and separation is set up for microbiological applications in water analysis. Magnetic nanoparticles coupled with specific antibodies to E. coli and to other relevant microorganisms are delivered from Miltenyi Biotec GmbH in cooperation. Protein microarrays are another focus for the quantitative detection of the microorganisms. A sandwich immunoassay is developed in which primary antibodies are immobilized in a microarray arrangement at slides. The positive signal of a present microorganism is generated by chemiluminescence if a second antibody binds to the microorganism at the surface. The signal is detected with a CCD camera.

First steps will be the development of effective surface chemistry for the bioactivity of the immobilized antibodies and the adaptation of the MACS technology of Miltenyi Biotec GmbH for microbiological purposes. The quantification of the microorganisms with standard methods and the use of real samples will be carried out in a close cooperation with the Stadtwerke München. The new microbiology lab and the concepts are the starting point for the new research field at the IWC.
(*M. Seidel*)

2 Publications of Present Members of the IWC

2.1 Journal articles (reviewed)

M. Ammann, U. Pöschl, Kinetic Model Framework for Aerosol and Cloud Surface Chemistry and Gas-particle Interactions: Part 2 - Exemplary Practical Applications and Numerical Simulations, Atmospheric Chemistry and Physics Discussions, 5 (2005) 2193-2246

T. Baumann and C. J. Werth; Visualization of Colloid Transport through Heterogeneous Porous Media using Magnetic Resonance Imaging, Coll. Surf. A, 265 (2005), 2–10

S. Eremin, D. Knopp, R. Niessner, J. Hong, S.-J. Park and M. Choi; High Throughput Determination of BTEX by a One-step Fluorescence Polarization Immunoassay. Environ. Chemistry 2 (2005) 227-230

T. Franze, M. Weller, R. Niessner and U. Pöschl; Protein Nitration by Polluted Air. Environ. Sci. Technol. 39 (2005) 1673-1678

N. Ivleva, R. Niessner and U. Panne; Characterization and Discrimination of Pollen by Raman Microscopy. Anal. Bioanal. Chem. 381 (2005) 261-267

M. Kiening, R. Niessner and M. Weller; Microplate-based Screening Methods for the Efficient Development of Sandwich Immunoassays. Analyst 130 (2005) 1580-1588

M. Kiening, R. Niessner, E. Drs, S. Baumgartner, R. Krska, M. Bremer, V. Tomkies, P. Reece, C. Danks, U. Immer and M. Weller; Sandwich Immunoassays for the Determination of Peanut and Hazelnut Traces in Foods. J. Agric. Food Chem. 53 (2005) 3321-3327

D. Matschulat, A. Deng, R. Niessner and D. Knopp; Development of Highly Sensitive and Specific Monoclonal Antibody Based ELISA for Benzo[a]pyrene. Analyst 130 (2005) 1078-1086

A. Messerer, D. Rothe, R. Nießner und U. Pöschl; Kinetische Betrachtungen und Modellrechnungen zur kontinuierlichen Regeneration von NFZ-Dieselrußpartikel-abscheidesystemen. Chemie-Ingenieur-Technik 77 (2005) 881-886

U. Pöschl, Y. Rudich, M. Ammann, Kinetic Model Framework for Aerosol and Cloud Surface Chemistry and Gas-Particle Interactions: Part 1 - General Equations, Parameters, and Terminology, Atmospheric Chemistry and Physics Discussions, 5 (2005), 2111-2191

U. Pöschl, Atmospheric Aerosols: Composition, Transformation, Climate and Health Effects, Angewandte Chemie International Edition, 44 (2005), 7520-7540

U. Pöschl, Atmosphärische Aerosole: Zusammensetzung, Transformation, Klima- und gesundheitseffekte, Angewandte Chemie, 117 (2005), 7690-7712

H. Prestel, L. Schott, R. Niessner and U. Panne; Characterization of Sewage Water Plant Hydrocolloids Using Asymmetrical Flow Field-Flow Fractionation (AF4) and ICP-Mass Spectrometry (ICP-MS). Water Res. 39 (2005) 3541-3552

M. Rampfl, K. Breuer and R. Niessner; Bestimmung von primären, sekundären und tertiären aliphatischen und aromatischen Aminen sowie Stickstoff-Heterocyclen und Alkanolaminen in Luft via HPLC-ESI-MS. Gefahrstoffe-Reinhaltung der Luft 65 (2005) 293-299

M. Rampfl, F. Mayer, K. Breuer, R. Niessner; Derivatization-free Analysis of Volatile Aliphatic and Aromatic Primary, Secondary and Tertiary Amines in Indoor Air by HPLC-ESI-MS, Proceedings: Indoor Air 2005, Volume II (2), 2144-2148

A. Sadezky, H. Muckenhuber, H. Grothe, R. Niessner and U. Pöschl; Raman Spectra of Soot: Spectral Analysis and Structural Information. Carbon 43 (2005) 1731-1742

E. Vogt, A. Held and O. Klemm; Sources and Concentrations of Gaseous and Particulate Reduced Nitrogen in the City of Münster (Germany), Atmos. Environ. 39 (2005) 7393-7402.

M. G. Weller, Optical Microarray Biosensors. Anal. Bioanal. Chem. 381 (2005) 41-43.

2.2 Journal articles (non-reviewed)

A. Strasser, R. Dietrich, E. Märtlbauer, B. Knecht, M. Weller and R. Niessner; Antibiotics Determinations with Biosensors, Deutsche Molkerei Zeitung 126 (2005) 48-51

2.3 Monographs

T. Baumann & R. Biber, Exothermal Reactions and Temperature Distribution in Bottom Ash Monofills, In: P. Lechner et al.: Waste Management in the Focus of Controversal Interests, 249–257, Vienna (Facultas) 2005

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), In: Results of the German Atmospheric Research Programme AFO 2000, R. Winkler (Ed.), pp. 40-43, Margraf Verlag, Weikersheim, 2005.

D. Knopp: Analysis of 2,4-Dichlorophenoxyacetic Acid in Body Fluids of Exposed Subjects Using Radioimmunoassay. In: J.L . Martinez Vidal, A.G. Frenich: Pesticide Protocols, 119–131 Totowa (Humana Press), 2005.

U. Pöschl, T. Franze, T. Fehrenbach, E. Mikhailov, U. McKeon, C. Schauer, A. Zerrath, Carbonaceous Aerosol Components: Chemical Composition, Reactivity, and Hygroscopicity (CARBAERO), In: Results of the German Atmospheric Research Programme AFO 2000, R. Winkler (Ed.), pp. 169-171, Margraf Verlag, Weikersheim, 2005.

M. G. Weller, Microarrays zur Analyse von Pflanzenschutzmitteln, Münchener Beiträge zur Abwasser-, Fischerei- und Flussbiologie, 2005, 155-171.

2.4 Conference Presentations

2.4.1 Oral Presentations

T. Baumann, Exothermal Reactions and Temperature Distribution in Bottom Ash Monofills, 1st BOKU-Waste Conference, 4.–6.4.2004, Vienna

T. Baumann, P. Fruhstorfer, T. Klein & R. Niessner, Colloid Transport in Contaminated Areas, KORESI Workshop, 19.-21.6.2005, Bad Herrenalb

T. Baumann und R. Biber, Exothermer Stoffumsatz in Schlackedeponien, Deponieforschung in Bayern, 8.6.2005, Augsburg

T. Fehrenbach, R. Niessner, U. Pöschl, Determination of Amino Acids and Proteins in Air Particulate Matter, 24th AAAR Conference, 17.-21.10.2005, Austin (USA)

D. Knopp, A. Deng, M. Letzel, M. Taggart, M. Himmelsbach, Q.-Z. Zhu, I. Peröbner, B. Kudlak, S. Frey, M. Sengl, W. Buchberger, C. Hutchinson, A. Cunningham, D. Pain, R. Cuthbert, A. Raab, A. Meharg, G. Swan, Y. Jhala, V. Prakash, A. Rahmani, M. Quevedo, R. Niessner; Immunological Determination of the Pharmaceutical Diclofenac in Different Matrices. Pacifichem 2005, 15.-20.12.2005, Honolulu, Hawaii, USA

U. McKeon, R. Niessner, U. Pöschl, Determination of Water-soluble Organic and Inorganic Atmospheric Aerosol Components, 24th AAAR Conference, 17.-21.10.2005, Austin (USA)

U. Pöschl, T. Fehrenbach, T. Franze, E. Mikhailov, U. McKeon, C. Schauer, A. Zerrath, Carbonaceous Aerosol Components: Chemical Composition, Reactitvity, and Hygroscopicity (CARBAERO), EGU 2nd General Assemply, 25.-29.4.2005, Vienna

H. Prestel, R. Niessner, and U. Panne: Die Slot outlet Technik: Ein neues Werkzeug zur Signalverstärkung in der asymmetrischen Fluss-Feldflussfraktionierung (AF4)? Wasserchemisches Kolloquium, 21.1.2005, Karlsruhe.

F. Tsagkogeorgas, D. Knopp, M. Ochsenkühn-Petropoulou, R. Niessner; Encapsulation of Proteins for Bioanalytical Purposes - Preparation of Nanometer-sized Silica Particles. IMA'05 (4th International Conference Instrumental Methods of Analysis, Modern Trends and Application), 2.-6.10.2005, Iraklion, Crete, Greece

M. G. Weller, High-speed Microarrays for the Detection of Antibiotics in Milk, 7. Statusseminar "Chiptechnologien", DECHEMA, 3.2.2005, Frankfurt.

2.4.2 Poster Presentations

M. Ammann, U. Pöschl, Kinetic Model Framework for Aerosol and Cloud Surface Chemistry and Gas-particle Interactions: Exemplary Numerical Simulations for Steady-state Systems, EGU 2nd General Assemply, 25.-29.4.2005, Vienna

M. Ammann, U. Pöschl, Kinetic Model Framework for Aerosol and Cloud Surface Chemistry and Gas-particle Interactions: Exemplary Numerical Simulations for Time-dependent Systems, EGU 2nd General Assemply, 25.-29.4.2005, Vienna

T. Baumann & R. Niessner, Transport of Colloids in Multiphase Systems, EGU 2nd General Assemply, 25.-29.4.2005, Vienna

T. Baumann, A. Keller, M. Auset & G. Lowry, Micromodel Study of Transport Issues during TCE Dechlorination by ZVI Colloids, AGU Fall Meeting, 5.-9.12.2005, San Francisco

S. Fabel, R. Niessner, M. G. Weller: Mikroanalysensystem mit Gassegmentierung für die Wirkungsbezogene Analytik, 4. Deutsches BioSensor Symposium, 13.-16.3.2005, Regensburg

T. Fehrenbach, T. Franze, S. Bhowmik, R. Niessner, U. Pöschl, Determination of Nitrated Proteins and Amino Acids in Fine Particulate Matter, ANAKON '05, 24.-29.4.2005, Regensburg

A. Held, A. Nowak, A. Wiedensohler, O. Klemm, Effective Deposition Diameter - A New Perspective on Size-Resolved Particle Deposition, European Aerosol Conference, 28.8. - 2.9.2005, Ghent.

D. Matschulat, A. Deng, R. Niessner, D. Knopp; Neue monoklonale Antikörper gegen Benzo[a]pyren, ANAKON '05, 24.-29.4.2005, Regensburg

U. McKeon, R. Niessner, U. Pöschl, Determination of Water-soluble Organic and Inorganic Aerosol Components, ANAKON '05, 24.-29.4.2005, Regensburg

M. Kiening, R. Niessner, M. Bremer, V. Tomkies, P. Reece, C. Danks, U. Immer, E. Drs, I. Leitzenberger, S. Baumgartner, R. Krska, M. G. Weller, Development of Rapid Immunoassays for the Detection of Peanut and Hazelnut Contaminations in Foods, ANAKON '05, 24.-29.4.2005, Regensburg

B. G. Knecht, M. Eiberle, R. Niessner, A. Strasser, R. Dietrich, E. Märtlbauer, M. G. Weller, High-Speed Microarrays for the Detection of Antibiotics in Milk, ANAKON '05, 24.-29.4.2005, Regensburg

U. Pöschl, E. Mikhailov, Water Interactions of Aerosol Particles Composed of Protein Macromolecules and Salts: Hygroscopic Growth, Microstructural Rearrangement, Electric and Kinetic Effects, EGU 2nd General Assemply, 25.-29.4.2005, Vienna

U. Pöschl, Y. Rudich, M. Ammann, Kinetic model framework for aerosol and cloud surface chemistry and gas-particle interactions, EGU 2nd General Assemply, 25.-29.4.2005, Vienna.

H. Prestel, R. Niessner & T. Baumann, Characterisation of Colloids in Manure using AF^4, EGU 2nd General Assemply, 25.-29.4.2005, Vienna

H. Prestel, W. Chen, R. Niessner, and U. Panne: Die Slot Outlet-Technik: Ein neues Werkzeug zur Signalverstärkung in der asymmetrischen Fluss-Feldflussfraktionierung (AF4)?, ANAKON '05, 24.-29.4.2005, Regensburg

H. Prestel, W. Chen, R. Niessner, and U. Panne: Die Slot Outlet-Technik als neue Methode zur Charakterisierung von Hydrokolloiden mittels asymmetrischer Fluss-Feldflussfraktionierung (AF4). Wasserchemische Gesellschaft, 1.-4.5.2005, Bad Mergentheim.

H. Prestel, R. Niessner, and U. Panne: Improvement of Asymmetrical Flow Field-flow Fractionation (AF4) Using Slot-outlet (SO) Technique. First Munich Conference on Field Flow Fractionation in Pharmaceutical Biotechnology, 6.-7.10.2005, Munich.

M. Yang, J. Lai, R. Niessner, D. Knopp; Detection of Endocrine Disrupting Chemicals (EDC) in Water: Synthesis of Artificial Receptors for Phthalate Esters using MIP Technology, ANAKON '05, 24.-29.4.2005, Regensburg.

2.4.3 Invited Lectures

D. Knopp: Application of Natural and Artificial Antibodies to Monitor Environmental Pollutants in Different Matrices. 14th International Scientific Congress, CNIC 2005, 27.-30.06.2005, Havanna, Cuba.

D. Knopp: Einsatz immunologischer Nachweisverfahren im Umweltbereich - eine kritische Bestandsaufnahme. AQS Fachtagung, Bayerisches Landesamt für Wasserwirtschaft, 26.04.2005, München.

R. Niessner, Future Trends & Challenges in Analytical Chemistry. BASF Ludwigshafen, 23.2.2005

R. Niessner, On line & In situ Chemical Analysis of Organic Aerosols. National University of Singapore, Dept. of Chemistry Seminar, 3.3.2005

R. Niessner, Laser or Antibodies - Best Friends of Analysts. GDCh-Kolloquium, Universität Giessen, 14.6.2005

R. Niessner, Selective Analysis by Antibodies and Photons Colloquium. Spectroscopicum Internationale, Antwerpen, 8.9.2005

R. Niessner, Laser or Antibodies - Best Friends of Analysts. Max-Planck-Institut für Polymerforschung, Mainz, 11.10.2005

R. Niessner, Trends in der Umwelt-Meßtechnik. IGAS-Jahrestagung, Berlin-Adlershof, 8.12.2005

H. Prestel and R. Niessner: Characterization of Hydrocolloids using Asymmetrical Flow Field-flow Fractionation (AF4). W.L. Gore & Associates GmbH, 27.1.2005, Putzbrunn.

M. G. Weller, Microarray-Biosensoren für die Detektion von Antibiotika und in der Allergiediagnostik, Interlab-Seminar "Mikrobiologische Analytik, Allergene und Kennzeichnung", Bayerisches Landesamt für Gesundheit und Lebensmittelsicherheit (LGL), 2.6.2005, Oberschleißheim.

M. G. Weller, S. Fabel, R. Niessner, Biochemische Detektion in der wirkungsbezogenen Wasseranalytik, GDCh-Jahrestagung, 12.9.2005, Düsseldorf.

M. Weller: Bioresponse-linked Instrumental Analysis, Workshop "Frontiers in Environmental Science", 7.10.2005, Kyoto, Japan.

2.4.4 Scientific Committee

T. Baumann, EGU 2nd General Assemply, 25.-29.4.2005, Vienna; Session Convener.

D. Knopp, IMA'05 (4th International Conference Instrumental Methods of Analysis, Modern Trends and Application), 2.-6.10.2005, Iraklion, Crete, Greece

R. Niessner, Gordon Research Conference on Chemical Sensors & Interfacial Design, 28.8.-2.9.2005, Oxford; Discussion 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, Bad Staffelstein, Straubing, Bad Tölz, Utting, Bad Wiessee, Bad Wimpfen

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

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

2.6 Bachelor Theses

Iris Peröbner (Molecular Biotechnology): Chemische Bestimmung des Arzneimittelwirkstoffes Diclofenac in biologischen Proben mittels ELISA - Verfahrensoptimierung

Luise Weigand (Molecular Biotechnology): Evaluierung eines neuen Benzo[a] pyren-Sulforhodamin B Tracers für die Entwicklung eines homogenen Fluoreszenzimmunoassays

2.7 MSc and Diploma Theses

Cand.phys. A. Bosnjak-Zoraja: Fundamentals of Photophoresis on Aerosols

Cand.chem. W. Chen: Optimization of the AF4-Slot-Outlet-Technique and its Application for Characterizing Sewage Water and other Hydrocolloids

Cand.phys. N. Dudeck: Interferometric Detection Techniques for Photoacoustic Tomography

BSc D. Kamble (GIST Singapore): Preparation of Heavy Metal Phosphate Tracer Colloids and its Application in Biofilm Reactors and in Environment

BSc G. Kassotakis (NTUA, Greece): Soot Oxidation in Open Filter Structures

BSc C. Nilsson (Environ. Engineering, Univ. Lund, S): Development and Validation of a Miniaturised Sorption Test

Cand.chem. T. Roßteuscher: Biofilm Observation with Photoacoustic Spectroscopy and Confocal Laser Scanning Microscopy (CLSM)

BSc F. Tsagkogeorgas, (NTUA, Greece): Preparation of antibody-doped nanometer-sized silica particles by reverse micelle and sol-gel processing

Cand.chem. M. Wiesmeier: Production and Characterization of Sol-Gel Materials for Immobilisation of Antibodies for Immunoaffinity Extraction of Cyanobacterial Toxins

Cand.chem. A. Wolter: Generation of Hapten Microarrays for Antibiotics Analysis

Cand.chem. Xin Yang: Raman Microscopical Studies on Changes of Elemental Carbon Crystallinity Under Oxidation at Elevated Temperatures

BSc Z. Sun (GIST Singapore): Generation of Anti-Arsenic Antibodies: Preparation and Characterization of Arsenic Conjugates

2.8 PhD Theses

Dipl.-Geol. M. Alte, Site Assessment, Securing and Remediation of a pH-Anomaly in Groundwater, TU München

Dipl.-Geol. D. Spangenberg, Electrokinetic Treatment of Water Work Residues, TU München

Dipl.-Ing. A. Messerer, Soot Particle Deposition and Oxidation in Catalysts for Commercial Vehicles, TU München

Dipl.-Chem. A. Zerrath, Analytics of Cellulose and Glucose in Ambient Aerosol Samples and Physical Aerosol Characterization with an Electric Low Pressure Impactor, TU München

2.9 Habilitation Theses

T. Baumann, Aquatic Colloids – Relevance for Transport Processes in Groundwater, Habilitation Thesis, TU München

U. Pöschl, Carbonaceous Aerosol Composition, Reactivity, and Water Interactions, Habilitation Thesis, TU München

3 Teaching, Colloquia, and Other Activities

3.1 Classes

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, Knopp, 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
Nutzung tiefer Geothermie	Schubert, Baumann
Biochemische und molekularbiologische Analysenverfahren in der Umweltanalytik	Knopp
Bioanalytical Methods in Environmental Analysis (National Technical University of Athens, Greece – ERASMUS/SOKRATES)	Knopp
Ringvorlesung “Biochemische Analytik” für BSc-Studiengänge Molekulare Biotechnologie und Biochemie (Thema: Immunologische Analytik)	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
Spurenanalytische Techniken	Niessner, Weller Haisch, Türler
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
Hydrogeologisches Praktikum II: Hydrochemische Methoden	Baumann, Niessner
Hydrogeologisches Praktikum III: Geländeübungen mit Kurs	Baumann, Haisch
Hydrogeologische und hydrochemische Exkursionen	Baumann, Niessner
Hydrogeologisches, hydrochemisches und umweltanalytisches Seminar	Baumann, Niessner

3.3 Institute Colloquia

PD Dr. Günter Tovar, Institut für Grenzflächenverfahrenstechnik, Universität Stuttgart: Preparation, Characterisation and Use of Molecularly Imprinted Nanospheres (18.1.2005)

Prof. Dr. Christiane Ziegler, Department of Physics, Universität Kaiserslautern: Nanobioanalytics - A Milestone in Medicine (19.1.2005)

Prof. Dr. Knut Schröder and Dr. Oyvind Mikkelsen, Dept. of Chemistry, Norwegian University of Science and Technology Trondheim, Norwegen: Continuous and Online Remote Monitoring of Heavy Metals (1.2.2005)

Dr. Hans-Peter Josel, R&D Diagnostics/Chemistry Roche Diagnostics GmbH, Penzberg: Luminescence Techniques for Diagnostics (15.2.2005)

Dr. Klaus Wittmaack, Institute of Radiation Protection, GSF Neuherberg: The Study of Sampling Artefacts: An Uncommon Approach towards a Better Understanding of Aerosol Properties and Composition (30. März 2005)

Prof. Yan Jin, University of Delaware: Retention and Transport of Viruses and Colloids in Undaturated Porous Media (22.4.2005)

Dr. Katrin Fichtl, Department of Microbiology, TU München: Polynucleotide Probe Based Enrichment of Bacterial Cells: Development of Probes for Species of Clinical Relevance (25.4.2005)

Prof. Arturo Keller, Univ. of California, Santa Barbara: Transport of Colloids in Unsaturated Porous Media: Explaining Large Scale Behaviour Based on Pore Scale Mechanisms (29.4.2005)

PD Dr. Roland Brock, Institute for Cell Biology, University of Tübingen: Peptidmicroarrays und fluoreszent markierte Zell-penetrierende Peptide - Funktionelle Proteomanalyse in vitro und in vivo (3.5.2005)

PD Dr. Oliver Hayden, Institut für Analytische Chemie, Universität Wien: Surface Imprinting Strategies of Thin Films (1.6.2005)

Dr. Christine Kranz, Georgia Institute of Technology, Atlanta/USA: Imaging with AFM-tip Integrated Microsensors (07.06.2005)

Prof. Dr. W. Knoll, Max-Planck-Institut für Polymerforschung Mainz: Supramolecular Interfacial Architectures for Optical Biosensing (10.6.2005)

Dr. Andreas Held, Institut für Landschaftsökologie, Klimatologie, Westfälische Wilhelms-Universität Münster: Time-of-flight Mass Spectrometry in Atmospheric Particle Exchange Measurements (4.7.2005)

Dr. Michael Seidel, F&E Engineering, Miltenyi Biotec GmbH, Bergisch-Gladbach: Miniaturisized Bioanalytical Methods for the Detection of DNA, Proteins and Cells (8.7.2005)

Prof. Dr. Claudia Steinem, Institut für Analytische Chemie, Universität Regensburg: Nano-BLMs: Development of Membrane Biosensors for the Detection of Channel Proteins and Pumps (28.7.2005)

PD Dr. Thorsten Reemtsma, Fachgebiet Wasserreinhaltung, Technische Universität Berlin: Environmental Application of High Resolution Mass Spectrometry - Elucidating the Composition of Fulvic Acids (24.10.2005)

PD Dr. Detlev Belder, MPI für Kohlenforschung, Mühlheim: Chemical Reactions and Analysis on Chip (2.11.2005)

PD Dr. Joachim Franzke, ISAS Institute for Analytical Sciences, Dortmund: Microplasmas and x-rays (11.11.2005)

Prof. Dr. Andreas Hierlemann, Institut für Quantenelektronik, ETH Zürich: CMOS as Technology Platform for Integrated Chemical and Biomicrosystems (29.11.2005)

Prof. Dr. Jiri Homola, Institute of Radio Engineering and Electronics, Academy of Sciences of the Czech Republic, Prag: Surface Plasmon Resonance Biosensors: Advances and Challenges (5.12.2005)

Prof. Dr. Karl Unterrainer, Institut für Photonik und Zentrum f. Mikro- und Nanostrukturen, Technische Universität Wien: Few-cycle THz Spectroscopy: A Tool for Spectro-imaging (13.12.2005)

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

Dr. Thomas Baumann

Bayer. Fachausschuß für Kurorte, Erholungsorte und Heilbrunnen	Member
Taskforce “pHOENIX” in the International Waste Working Group	Member
“AK Kolloide” in the Hydrochemical Society	Member

Prof. Dr. Dietmar Knopp

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

Dr. Ulrich Pöschl

Atmospheric Chemistry and Physics	Chief Executive Editor
European Geosciences Union	President of Atmospheric Sciences Division, Council Member

PD Dr. Michael Weller

Journal of Biochemical and Biophysical Methods	Editorial Board
Arbeitsgruppe ”Analytik von Stoffen in der Landwirtschaft” (SKLW)	Member
Fachausschuss ”Biochemische Arbeitsmethoden” (Wasserchemische Gesellschaft, GDCh)	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
1 384-channel washer, Biotek

4.2.6 Element Analytics

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

4.2.7 SEM/Microscopy/Colloid Sizer

1 SEM/EDX system
1 Polarisation microscope for phase analysis
1 Fluorescence microscope
1 Image analysis software for automated image processing
1 Inert gas glovebox
1 Laser Raman microscope, Renishaw (514 nm, 633 nm, 780 nm)
1 Zetaphoremeter, SEPHY

4.2.8 Sum Parameters

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

4.2.9 Aerosol Research

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

4.2.10 Microbiology

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

5 Staff 2005

Univ.-Prof. Dr. Reinhard Nießner

Dr. Thomas Baumann
Dr. Christoph Haisch
Dr. Andreas Held (from 9/05)
Dr. Natalia Ivleva
apl. Prof. Dr. Dietmar Knopp
Dr. Ulrich Pöschl (until 3/05)
Dr. Harald Prestel
Dr. Thomas Schmid (until 6/05)
Dr. Michael Seidel (from 10/05)
PD Dr. Michael G. Weller

Birgit Apel
Christine Beese (from 1/05)
Günter Dollinger (until 12/05)
Roswitha Glunz
Karin Koller (until 8/05)
Joachim Langer
Ramona Leube (until 5/05)
Susanne Mahler
Christine Sternkopf
Christa Stopp
Sebastian Wiesemann

Hatice Hazir
Mira Kolar

PhD Students

Dipl.-Geol. Matthias Alte (until 2/05)
Dipl.-Ing. Jackelyn Arágon-Gómez (until 4/05)
Dipl.-Chem. Christian Cervino (from 11/05)
Dipl.-Chem. Susanne Fabel
Dipl.-Chem. Tobias Fehrenbach
Dipl.-Ing.FH Clemens Helmbrecht (from 5/05)
Dipl.-Leb.Chem. Martin Kiening (until 5/05)
Dipl.-Chem. Bertram Knecht (6/05 - 11/05)
Dipl.-Met. Carsten Kykal (from 4/05)
Dipl.-Chem. Diana Matschulat (until 5/05)
Dipl.-Chem. Ulrike McKeon (until 11/05)
Dipl.-Ing. Armin Messerer (until 8/05)
Dipl.-Chem. Dieter Rothe (until 2/05)
Dipl.-Chem. Philipp Stolper (from 11/05)
Dipl.-Chem. Zhe Sun
Dipl.-Phys. Karin Zell (from 10/05)

External PhD Students

Dipl.-Biol. Melanie Maier (GSF)
Dipl.-Biol. Roman Radykewicz (GSF)
Staatl.gepr.Leb.-Chem. Michael Rampfl (IBP Holzkirchen)

Diploma Students/MSc Students

Ana Bosnjak-Zoraja (until 3/05)
Wei Chen (until 4/05)
Nikola Dudeck (until 1/05)
Leonard Hofmann (from 2/05)
Sebastian Jähme (from 7/05)
Deepak Kamble (until 1/05)
Georgos Kassotakis (until 2/05)
Christian Nilsson (4/05 - 9/05)
Caroline Peskoller (from 11/05)
Tobias Roßteuscher (from 5/05)
Fotios Tsagkogeorgas (until 2/05)
Markus Wiesmeier (until 5/05)
Anne Wolter (4/05 - 10/05)
Yang Xin (3/05 - 8/05)

External Diploma Students

Zhen Li (LaRoche) (from 9/05)

Bachelor Students

Iris Peröbner (Molecular Biotechnology)
Luise Weigand (Molecular Biotechnology)

Guests and Research Fellows

Christine Gigou (2/05 until 7/05)
Blazej Kudlak (4/05 until 8/05)
Prof. Dr. Evgene Mikhailov, University St. Petersburg (from 11/05)
Dr. Minli Yang, University Peking
Prof. Dr. Hwang Gab-Soo, University Korea (until 3/05)
Thomas Willingham, University of Illinois (6/05)

Student Assistants

Kirsten Langfeld (3/05 - 5/05)
Stefan Preißer (from 9/05)
Yvonne Monsorno (until 2/05)
Laura Toops (7/05 until 11/05)