



Institute of Hydrochemistry

**Chair for Hydrogeology,
Hydrochemistry and
Environmental Analytical
Chemistry**

Annual Report

2001



Institute of Hydrochemistry
Chair for Hydrogeology, Hydrochemistry and Environmental Analytical Chemistry
Technische Universität München
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Editor: Dr. Thomas Baumann

Editorial

Dear Friends and Colleagues,
for the first time our annual report is published in English to acknowledge our international readership. Following the current mainstream in university teaching, we participated this year in efforts to establish new bachelor/master courses in chemistry and geology at the Technische Universität München (TUM). This is in part a reaction on the tremendous breakdown in the number of diploma and/or PhD candidates. In the early nineties, we had about 30 PhD students per year working at the IWC. At present, this number dropped to 19 PhD students, a similar effect is observed for the diploma students. In former times, we reported on 13 completed diploma theses per year. In 2002, we host only one diploma student. Bad times? Not really, I believe, it rather will be the ultimate challenge to do innovative research in analytical chemistry. Maybe we have to recruit more outside Germany resp. Europe for new members of our club. In addition, we will keep the ship afloat with more PostDocs and visiting scientist, especially from Asia. On the other hand, we never had before such an intensive scientific output as it is observed now. The movement into high-ranking journals for publication is seen as a must and the appearance of 10 papers in 2000 and 2001 in *Environ. Sci. Technol.*, *J. Phys. Chem.* and *Anal. Chem.* is a good sign for this. In the last year, Dr. M.G. Weller successfully finished his habilitation. Congratulations to him!

After heading the institute in Munich-Grosshadern for 12 years now, the institute is well established. One might say that in the meantime even analysts know what balneology in the institute's name means. It seems now time for a further evolution: The "Geozentrum", a merger between the Geology of LMU and TUM is in the focus of many spirited discussions. In addition, the Faculty of Chemistry in Garching at TUM is under a reconstruction. Some institutes are supposed to disappear in future, but time will show. Nothing is more persistent than water – it can only be used, but not consumed.

On behalf of the whole institute, I would like to express my sincere thanks to all friends, especially to the Kreis der Freunde des Instituts für Wasserchemie & Chemische Balneologie, and all the funding organisations who supported us in 2001. More than 4.8 million DM funding is a benchmark for many other institutes. Finally, I would like to thank all staff at our institute for their support and ongoing excellent work.



Reinhard Nießner
Head of the Institute

1 Research

1.1 Hydrogeology

1.1.1 Visualization of Colloids in Porous Media With MRI

Funding: IWC TUM

Cooperation: University of Illinois at Urbana-Champaign (Prof. Werth)

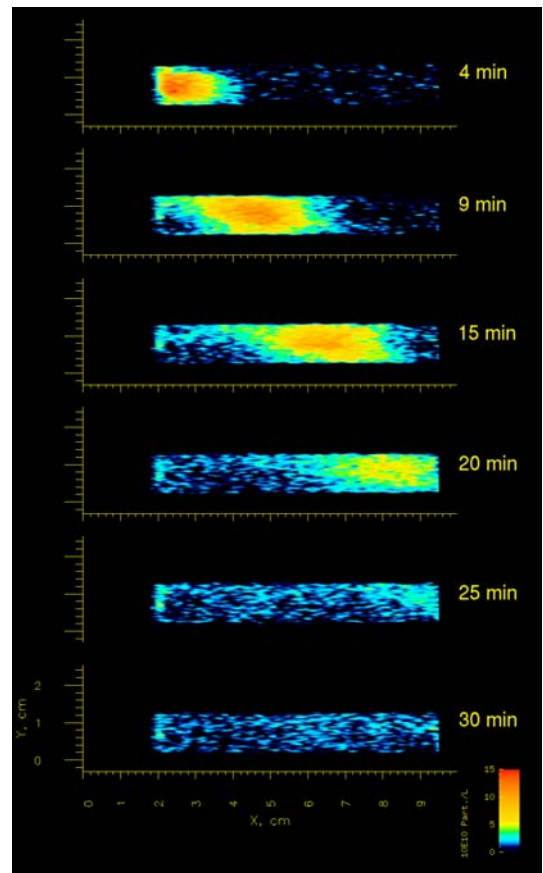
Colloid transport can significantly impact the fate of contaminants in subsurface environments. Colloid transport is very sensitive to hydrochemical and hydrodynamic conditions. Conventional methods to investigate colloid transport often involve column studies, where colloid concentrations are measured at the column effluent or at selected points along the column length. Unfortunately, this approach does not distinguish how spatial and temporal changes in hydrochemical and hydrodynamic conditions affect colloid transport. In order to examine the effects of these changes, non-invasive techniques have to be applied.

One promising non-invasive technique is magnetic resonance imaging (MRI). MRI allows the visualisation of dynamic processes in porous and fractured media, including the transport of colloids. During a six-month sabbatical leave of T. Baumann at the University of Illinois the transport of superparamagnetic colloids through columns filled with silica gel was quantified using MRI. Two columns (1 cm ID by 5 cm length) were packed, each with a core of fine-grained silica gel surrounded by a shell of coarse-grained silica gel. In column #1, 600-850 μm silica gel was surrounded by 850-1000 μm silica gel. In column #2, 250-600 μm silica gel was surrounded by 850-1000 μm silica gel. Both columns were continuously purged with deionized distilled water at 9 mL/h, and colloids were introduced as 0.11 mL pulses. During colloid transport images were taken every three minutes with a spatial resolution of $0.2 \times 0.2 \times 1 \text{ mm}^3$.

MRI images of column #1 showed that colloid transport in the core and shell was not distinguishable. However, colloid transport was slightly faster along the top of the column. T1-weighted images showed that small variations in the packing density of silica gel caused this effect. MRI images of column #2 showed that colloid transport in the core was much slower than colloid transport in the shell. Colloid exchange between the shell and the core was also observed, and this occurred to a greater extent at one location. T1-weighted images did not reveal variations in packing density along the column; so it is not clear why preferential exchange between the core and shell occurred.

Colloid transport velocities were calculated from the images.

In agreement with the images, velocities for column #1 increased from the bottom to top of the column, and velocities for column #2 were greater in the shell than in the core. Velocities from images were also compared to velocities from conventional experiments where colloid concentrations were measured at the column effluent. While comparable, velocities from the latter mask many of the complexities that control the overall rate of colloid transport. Since these complexities can give rise to very different transport behaviour, it is critical to understand their effects in real systems. Hence,



MRI is a powerful technique that has the ability to elucidate many of the small-scale processes that lead to the behaviour of colloids in the field.

(*T. Baumann*)

1.1.2 Applications of MRI in Hydrogeology

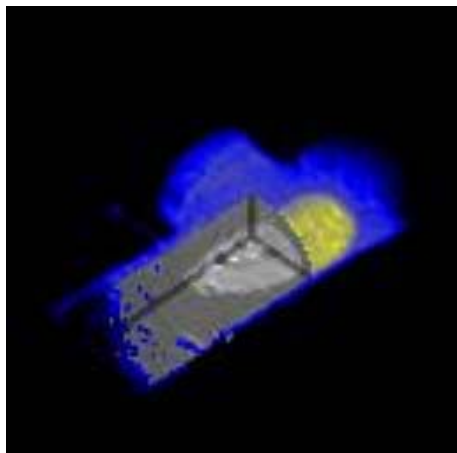
Funding: DFG, Ba1592/1-1

Cooperation: Department of Neuroradiology Großhadern, LMU, Department of Radiology, University of Ulm

Present knowledge on the fate and propagation of contaminants in aquifers relies mainly on column experiments in which the outflow from a sediment column with known time profile of the inflow concentrations is studied as a function of time. From these time profiles, the processes governing transport, filtration (or sorption) and remobilisation of the contaminants are computed on the basis of mathematical models for the flow and binding processes in the columns. As neither flow profiles nor concentrations profiles over the column are actually known in such an experiment, the correctness of the assumed model cannot be directly verified.

Magnetic Resonance Imaging (MRI) is an excellent experimental tool for spatially resolved non-destructive studies of the stage of water and the distribution of contaminants within a sediment column. In the framework of the ongoing project, we have shown the potential of MRT to study various processes such as the binding of sorptive heavy metal ions in sand sediments under water flow:

- Enrichment of ions from a dilute solution on the pore surfaces
- Traces left by the propagation of a locally injected higher concentration of heavy metal ions with the water flow
- Remobilization of adsorbed heavy metal ions upon changing hydrochemical conditions.



The amounts of heavy metal ions used in these studies were typically single-digit mg-quantities. Of the distribution of these ions, 3-D volume data with a spatial resolution of less than 10 mm^3 and with a temporal resolution of minutes could be achieved. Secondly the propagation and dissolution of non-aqueous-phase liquids (NAPL) in sand sediments under water flow was addressed. In these experiments, a quantity of about 50 mL NAPL was injected into the column and its propagation with the water flow was observed. For some NAPL such as MTBE a rapid disintegration of the injected liquid into small droplets was observed in the MRI experiments while other NAPL were found to propagate as macroscopically coherent phase and dissolve mainly from the interface of the surrounding water phase. The dissolution of NAPL quantities could be monitored down to the sub-mL range in these experiments.

Direct observation of substance profiles during a column transport experiment not only permits the identification of possible local deviations from model assumptions but also enable direct studies of the action of inhomogeneity and of non-equilibrium processes in the column. These possibilities offer an interesting potential for fast laboratory-scale tests of remediation measures or for risk assessment studies on such models.

(*N. Nestle*)

1.1.3 Exploration of Ground Water and Mineral Water

Funding: State of Bavaria

As a safety measure for the mineral waters of Sibyllenbad/Opf. an intense hydrochemical monitoring program for the existing wells was launched. Furthermore the search for new mineral water occurrences has been started. In addition to the interpretation of aerial photographs, VLF-measurements and geoelectrical soundings (both carried out by Prof. Ernstson) were used to identify promising locations for well drilling. The measurements were delayed because of a lacking cooperation of the site owners. The results are expected during spring 2002.

Still massive iron hydroxide deposition takes place at the radon containing wells, causing costly cleaning procedures. We are therefore looking for a replacement of these wells in the near future.

(M. Baumann)

1.1.4 Exothermal Reactions in MSWI Bottom Ash Landfills

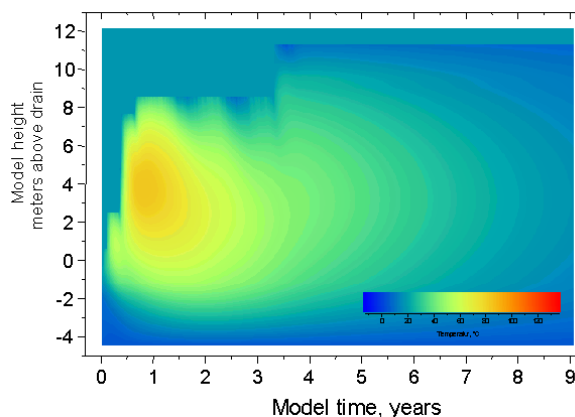
Funding: BayFORREST F158

Until the 1970s, bottom ash from the municipal solid waste incineration was believed to be almost inert, but since then several studies have shown that exothermic reactions may cause a temperature increase in the landfill of up to 90 °C. There are reported several exothermic reactions in bottom ash material. The most decisive reactions for the temperature increase in the stored bottom ash are the corrosion of iron and aluminium, the hydration of lime (CaO) and the carbonatization of portlandit (Ca(OH)₂).

Although the exothermic reactions in the bottom ash are well known, the speed of reaction and its amount of the specific heat are still unknown. We have shown, that the main temperature increase due to the exothermic reactions have a time scale of 2 to 3 months and found an initial specific heat of 26 W/m³ bottom ash stored for 4 weeks prior to disposal.

Assessing the thermal capacity of the residues is essential since bottom ash has been deposited in landfills with poor landfill liner systems in Europe and in other countries during the last decade. In the US, bottom ash was commonly landfilled without processing, even though metals and other materials can be recovered by magnetic separation and screening. In some European countries (e.g. Germany, The Netherlands and France) bottom ash is partly reused (about 60 %) in road construction or as raw material for the ceramic and cement industry, whereas in Switzerland almost 100 % of the bottom ash is disposed in landfills.

High temperatures at the base of a landfill endanger the stability of the landfill liner system (flexible membrane liner, FML, and mineral clay layer). Temperatures above 40 °C may affect the stability of the FML (made of High-Density-Polyethylene) due to depolymerisation and oxidation. Sudden rupture of the FML is a possible consequence. Due to a diffusive transport of water and water vapour along the temperature gradient in the mineral clay layer, the clay barrier desiccates and fails to retain leachate. In order to prevent thermal damage on the liner system, it is necessary to minimize



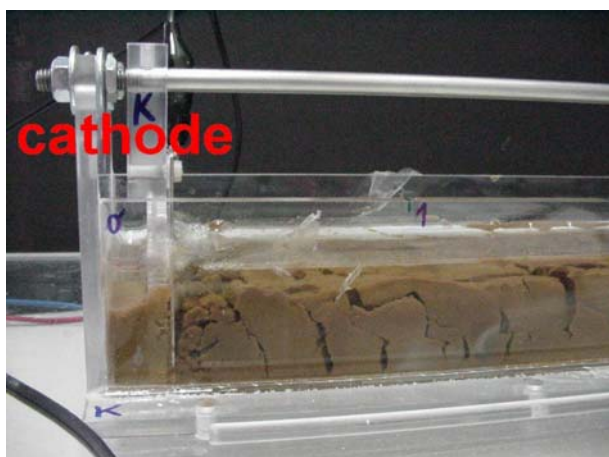
temperature development in the landfill. There are several factors such as the ambient temperature, the surface-to-volume ratio and the deposition temperature of the bottom ash influencing the temperature development in a landfill. A numerical model incorporating basic concepts from chemistry and physics was developed to simulate the spatial and temporal distribution of heat in a bottom ash landfill. This objective was accomplished in two steps: (1) the observation of the temperature development in a bottom ash landfill under several modes of emplacement, and (2) the development of a heat generation and transport model and coupling this with the obtained data from the landfill field experiments. With this numerical simulation model, we have a possibility to predict the temperature development in a bottom ash landfill regarding several modes of emplacement.

(*R. Klein, C. Speiser*)

1.1.5 Electrochemical Cleanup of Water Treatment Residues

Funding: BayFORREST F179

During drinking water treatment organic contaminations and heavy metal ions are removed from the raw water by flocculation and filtration. The contaminants accumulate in the residual sludge which accrues after the backfiltration of the sand filter.



The concentrations of heavy metals and AOX often do not meet the requirements for a direct discharge of the sludge into the sewer, although this could be one of the more advantageous disposal pathways. First, an addition of metal salts for the phosphate precipitation is not necessary due to the relatively high iron-content in the waterwork residues. An addition of lime-milk is also mostly not necessary due to the high lime concentration in the waterwork sludges. Similarly the desulphurisation of the sewage gas is not needed due to the high iron concentrations in the sludges. A consequence of the waiving of precipitants is a reduction of the salinisation of the recipient stream.

In Germany, approximately 125.000 t of waterwork sludges (dry matter) are produced per year. Roughly 50 % of these sludges are deposited on landfills, 7 % are fed into the sewer or directly into the to wastewater treatment plants, 4 % are used for cement and brick production, 16 % are used in different ways, whereas for the rest of 23 % the utilisation is unknown.

The objectives of this project are the geochemical and mineralogical characterisation of waterworks residues and the development of an electrokinetic method for the removal of heavy metal ions and organic contaminants in order to meet the standards for a subsequent use as an additive for waste water treatment plants.

The treatment technique is based on electrophoresis, electroosmosis and electrochemical processes at the electrodes. First experiments with synthetic and real sludges suggest that a cleanup of the waterwork sludges with electrokinetic methods is possible. (*D. Spangenberg, A. Reisinger*)

1.1.6 Statistical Methods for the Assessment of Leachate Concentrations at the Point of Compliance

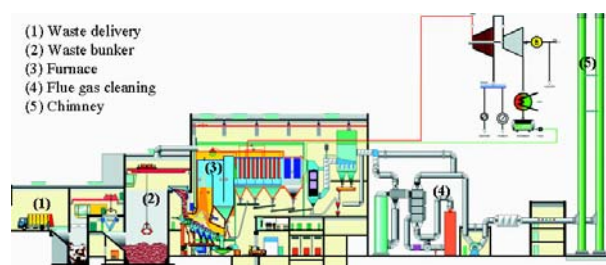
Funding: BMBF 02WP0175

The combustion of 14.000.000 tons of domestic waste in 61 German incineration plants (MVA) generates about 600.000 t of bottom ash in the Federal Republic of Germany per year. The bottom ash consists of a heterogeneous mixture of silicates, carbonates, oxides, sulfides, sulfates and salts. During the discharge from the incinerator, the contact of the dry bottom ash with the water of the quencher causes the formation of several mineral phases. Under specific conditions of temperature and pressure, a thermodynamic equilibrium can be partly realised. Under atmospheric conditions, these mineral phases are not stable and adapt according to their new environmental condition. After the three-month storage period prior to further recycling, bottom ash can be used as a recycling material in road construction or in landscape gardening.

After a storage time of three weeks the bottom ash can be deposited in a landfill. During the temporary storage, but particularly during the final storage in the landfill, precipitation causes leaching in the deposited bottom ash. For the quantification of the eluted elements the ionic concentration was determined in the seepage water from a bottom ash landfill and elutions were evaluated according to German DIN 38414-S4 (DEV S4) standard. According to the German Bundes-Bodenschutz-Verordnung (BBod-SchV 1999) the heavy metal ions are examined in this work.

It could be shown in the leachate of the aged bottom ash that there is a reduced mobilisation of heavy metals with rising storage time of the bottom ash on the landfill. This phenomenon is accompanied by a decreasing pH value in the same period of time. During the carbonatization of the bottom ash, which rises with increasing storage time, we observed an integration of the heavy metals into the newly formed insoluble carbonate phases. Also the leachate obtained from container storage underlines the reduced mobilisation of heavy metals with rising carbonisation.

(R. Klein)



1.1.7 In Situ Monitoring for Soil and Water by Infrared Sensing

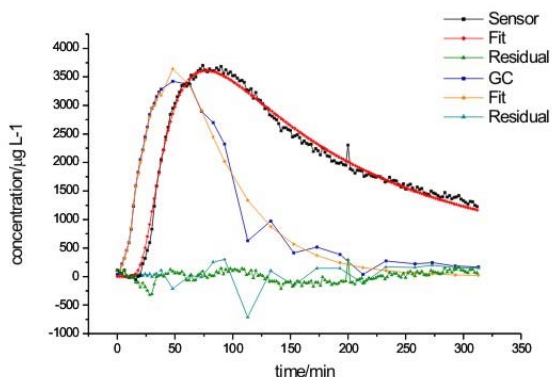
Funding: EU EVK1-CT-1999-00042

Cooperation: Fraunhofer-Institut für Physikalische Messtechnik, Freiburg; Technische Universität, Wien; Universität für Bodenkultur, Wien; Tel Aviv University; Université de Rennes; CSIC, Barcelona

In spite of numerous European efforts for the reduction and prevention of waste, the production still increases. Nearly 60 % of domestic waste and 68 % of hazardous waste are still deposited in landfills. Many of these landfills are presently not state of the art. This means they are not equipped with flexible membrane linings, mineral base linings or seepage water collection and treatment systems. One can assume that ground and surface water in the surrounding of landfills is exposed to the risk of contaminations for a long time. Consequently there are increased requirements for a continuous control and surveying system of landfill contaminations. Not only landfills, but also abandoned waste sites need to be screened and monitored for possible release of organic matter.

Within the scope of the IMSIS project (In Situ Monitoring of Landfill Related Contaminants in Soil and Water by Infrared Sensing) a fibre-optic sensor system for

the detection of organic pollutants (BTEX, PAH, etc.) in groundwater and seepage is developed. Besides, the IMSIS system should be used for the screening of landfills and abandoned sites.



The IWC has to provide laboratory and pilot scale facilities for testing the sensor system and to select sites which are adapted for real world experiments with the IMSIS system. These possible fields of application have to be presented and the legal issues for measuring campaigns have to be set. The contaminated sites have to be characterized hydrochemically and hydrogeologically, as well as the representativeness of the sensor data for the total contamination has to be evaluated. Respectively the response behaviour of the IMSIS sensor system for short and long term concentration changes has to be verified. Furthermore, the long term stability of the system - especially the composition and the effects of organic and inorganic coatings - has to be investigated. To what extent even colloidal transport of contaminants could be seized with

a fibre-optic device, is one of the main focuses of these studies.

After a calibration of the detecting unit, it is possible not only to prove the existence of organic pollutant groups like VOC, BTEX, PAH, phenols or alike. Rather there is the opportunity to "see" single substances like TCE or DCB, or to figure out the information for single substances from the measured spectral data, by using a newly created spectral database.

The IMSIS sensor system comprises a portable Fourier transform infrared spectrometer (FT-IR), coupled with a silver halide fibre-optic cable leading to the sensorhead and back to the detection unit of the spectrometer. The detection limit for the sensor system is in the mg/L range, while the enrichment of the pollutants within the polymer coating of the fibre takes a few minutes. The sensorhead should be inserted in monitoring wells and be placed 10-20 m below the ground surface both in varying depths and at different places within one site.

The IMSIS system is to be used for short- to medium-term surveillance of groundwater monitoring wells, or be fixed for long-term surveillance. In addition, the system is to be upgraded at existing sites and to be installed at new built landfills in Europe.

Particularly at the planning of remediation actions and the critical phase of decontaminations, a flexible field measuring system is useful for a fast and steady contribution of analytical data.

(M. Alte, M. Sarnes)

1.2 Hydrochemistry

1.2.1 Photocatalytic Atrazine Degradation by Synthetic Minerals, Atmospheric Aerosols and Soil Particles

Funding: BayFORUV C2

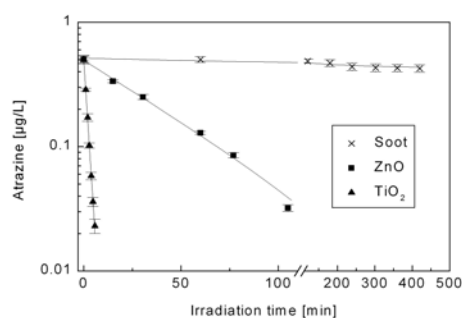
In the last two decades, photocatalytic degradation of harmful pollutants by irradiated particles has received considerable attention. Most investigations so far were carried out with aqueous suspensions of TiO_2 , but other mineral particles such as ZnO or Fe_2O_3 also showed photocatalytic activity. Taking into account that there is a wide range of mineral particles in the environment (soils or atmospheric particles like dust, fly ash, volcanic ash), it can be assumed that photocatalytic reactions induced by solar radiation may occur in the natural environment. Experimental studies on photocatalytic reactions using real atmospheric aerosols or soil samples are just beginning. Therefore, it is unclear whether photocatalysis by environmental particles contributes to the abiotic degradation of persistent organic substances, e.g. like the herbicide atrazine, a representative substance out of the class of triazine herbicides.

In this study the photocatalytic degradation of atrazine was studied on model minerals and real particle samples. The model minerals can be divided into known photocatalysts (TiO_2 , Fe_2O_3 , ZnO , ZnS) and mixed oxides (FeTiO_3 , SrTiO_3). The real samples were chosen to cover a range of typical natural and anthropogenic environmental particles (sand, soot, dust, fly ash, volcanic ash). Suspensions of the different particle systems were irradiated with a sun simulator, and the atrazine degradation was monitored by direct, competitive ELISA (enzyme-linked immunosorbent assay). Atrazine detection by ELISA proved to be an useful analytical tool due to low cross-reactivity of atrazine metabolites and high sensitivity with detection limits in the low ng/L range. The atrazine degradation followed first order kinetic and the obtained rate coefficients were compared with the rate of direct photolysis.

Atrazine was rapidly photodegraded by known photocatalysts like TiO_2 , ZnO and ZnS , whereas mixed oxides and iron containing compounds exhibited no significant photocatalytic activity. Atrazine degradation by using irradiated Niger sand colloids was 40 % faster than by direct photolysis. Irradiation of soot particles or Arizona test dust did not enhance the degradation of atrazine, the rate coefficients were within the error bars of direct photolysis. During the irradiation of volcanic ash and fly ash particles no significant atrazine degradation was measured. It can be concluded, that photocatalysis by environmental particles does not enhance the abiotic degradation of atrazine.

Due to the known rapid photocatalytic degradation of volatile organic compounds by irradiated aerosol particles a faster degradation of atrazine on irradiated real particulate matter has been expected. The findings of this study do not confirm these hypotheses. However, the obtained results are in agreement with the low photocatalytic activity of soils and fly ash concerning atrazine degradation reported before. The atrazine half-lives reported for different soil suspensions or thin layers are not significantly shorter than direct photolysis in water.

(M. Lackhoff)



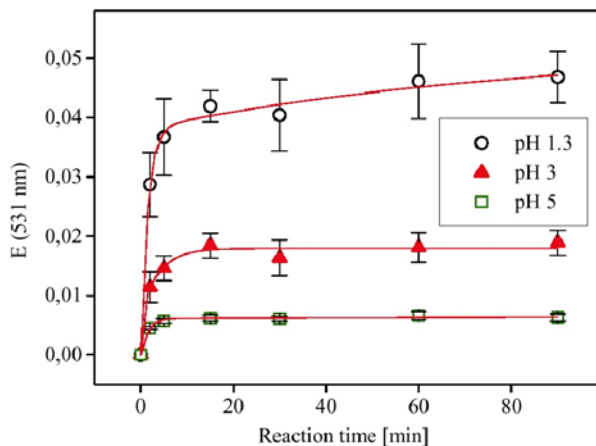
1.2.2 Investigation of the Hydroxyl Radical Formation in Natural Humic Systems

Funding: IWC TUM

Cooperation: Institute of Environmental Chemistry, Heidelberg (Prof. Schöler)

The formation of hydroxyl radicals in natural aqueous humic acid systems was investigated. The aim of this studies was to demonstrate the formation of this radical species in those systems. It is assumed that the formation of natural organohalogen compounds is initiated by a reaction between the salt content of the soil and radicals.

In contrast to the data available from the literature a radical formation was followed over a total period of 90 min. It was found that the formation at different pH values takes place almost over the whole period.



Furthermore the concentration of this radical species was quantitatively determined. For this purpose the 2-deoxy-D-ribose (2-DR)-method was used. This method allows the capture of all formed radicals by adding the sugar to the investigated solution and is very sensitive (the limit of detection was determined to be approximately $4 \cdot 10^{-11}$ mol/L). By the reaction between hydroxyl radicals and 2-DR malondialdehyde is released. The aldehyde is verified in the next step by a reaction with thiobarbituric acid in a trichloroacetic acid solution forming a pink product which can easily be measured spectroscopically. By using sonolysis as a source for hydroxyl radicals the actual concentration can be determined by Fricke dosimetry. By comparing the measured absorption of the 2-DR-method the actual radical concentration in the system can be calculated.

The main results found in these investigations are: the formation of these radical species is influenced by two parameters of the system, the iron(II) concentration and the oxygen content. Since humic acid (and all other natural occurring soils) contain different concentration of iron and of course oxygen the proved radical formation takes place in all of these systems.

In the investigated systems the ratio between the concentration of the formed hydroxyl radicals and the humic acid content (both given in mg/L) was determined to be in the range of about 10^{-4} . This means that the formation of hydroxyl radicals and beyond the formation of halogen radicals can not be neglected as a potential source of organohalogen compounds.

(M. Seiss)

1.2.3 On-line Detection of Heavy Metals Using Laser-induced Fluorescence Spectroscopy and FIA: The Field Experiment Vollert-Süd

Funding: BMBF 02WS9732/4

Cooperation: TU Hamburg-Harburg (Prof. Förstner)

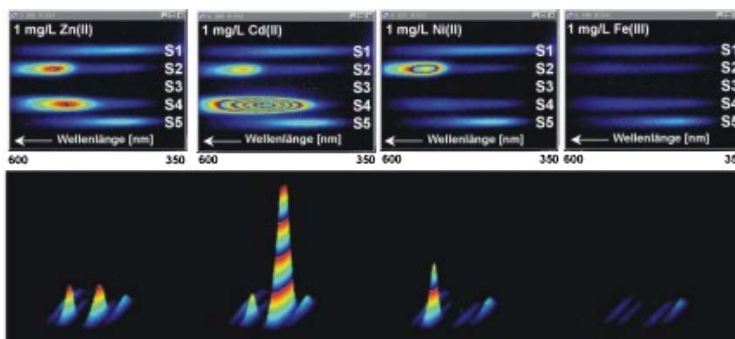
A mobile, fiber optic sensor system has been developed to detect dissolved heavy metal ions. This sensor combines laser-induced fluorescence spectroscopy (LIFS) of suitable metal-ligand complexes with flow injection analysis (FIA). The samples are injected into five sensor modules, where different complexing agents form complexes with various heavy metal ions. These complexes are excited by a nitrogen laser to produce fluorescence. The detection unit consists of a spectrograph with an intensified

CCD camera, which enables a simultaneous detection of different metal ions at the ppb level. It has been shown that the FIA sensor system has good reproducibility and allows a high sample throughput.

The following chelators were employed: Bathophenanthroline, BTC-5N, chromotropic acid, 3,3'-Dihydroxybipyridine, Fura-2, neocuproine, Newport Green™ and salicylic acid. These complexing agents were tested for their suitability to detect Pb^{2+} , Cd^{2+} , Hg^{2+} , Zn^{2+} , Ni^{2+} , Cu^{2+} , Be^{2+} , and Fe^{3+} . Preliminary examinations have been carried out in tap, river, and sea water for single-element and for multielement determinations of two, three and four various metal ions in the $\mu\text{g}/\text{L}$ to mg/L range.

In addition the chelators were employed for the on-line detection of heavy metals in a field experiment at the lake Vollert-Süd in Saxony-Anhalt. To investigate the effect of a natural Phillipsite barrier on the transfer of heavy metals from a highly contaminated sediment, the sensor was coupled with a new dialysis sampler, which has been developed by the TU Hamburg-Harburg. During a period of 15 months heavy metal concentrations have been measured and compared with those from the developed sensor system. Additionally, established instrumental methods (AAS, TXRF, ICP-MS) have been carried out off-line. The results show that no heavy metals have been mobilized from the sediment and demonstrate the usefulness of the developed sensor system for field measurements.

(H. Prestel)



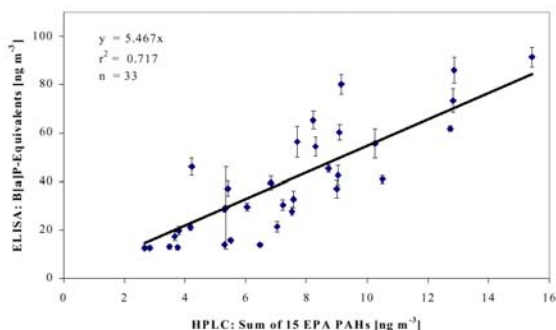
1.3 Bioanalytics I

1.3.1 Automated Immunoassay System for Continuous Air Safety Control (AISAC) and its Application to Air Pollution and Aero-allergen Monitoring

Funding: EU IC15-CT-98-0322

Cooperation: Institute Pasteur (Paris, France), University Pècs (Pècs, Hungary), Academy of Sciences (Prague, Czech Republic), EXBIO Praha (Prague, Czech Republic)

The main objective of this project is the detection and analysis of some major aero-allergens and organic pollutants that are either toxic by themselves or are cofactors of allergenicity. The project involves truly complementary partners which are specialized in different fields. There is an increasing evidence that air pollutants can constitute an important trigger in the development of allergic diseases. Whereas gaseous pollutants are now well detected and quantified by automated equipments, aerosols of dust or pollen particles and organic compounds are not easily analysed currently.



Pollutants resulting from burning of fossil fuels and automobile exhaust gas are especially suspicious of causing allergic airway diseases. The potential of polycyclic aromatic hydrocarbons (PAHs) to alter the immune function of human beings has been well established in the past. Until now only very limited data are available on the usefulness of immunological methods (immunoassays) for the determination of organics in airborne aerosols. Therefore, we have generated a monoclonal antibody for PAHs on the base of a new benzo[a]pyrene immunogen and have developed an ELISA. The antibody has a range of use-

ful and interesting properties which make it a valuable analytical tool. For example, its tolerance of certain amounts of organic solvents is an important prerequisite for analysis of PAHs in sample extracts. The broad selectivity of the assay, especially for the higher annelated compounds makes it useful for the determination of a PAH sum parameter. Real samples of particulate matter were collected at a high traffic crossing. The filters were extracted and the extracts analysed both by ELISA and traditional HPLC method. The approximately five-fold overestimation observed for the ELISA compared with the sum of 15 EPA PAH concentration (without acenaphthylene) is probably a result of the recognition of other polyaromatic compounds in aerosol extracts by the antibodies and, therefore, their contribution to the ELISA signal. The immunochemical method is a cost-effective alternative to large-scale screening, because as several samples can be determined in parallel and it might, therefore, be of interest for initial screening of air quality, and for comparison with data obtained from routine monitoring.

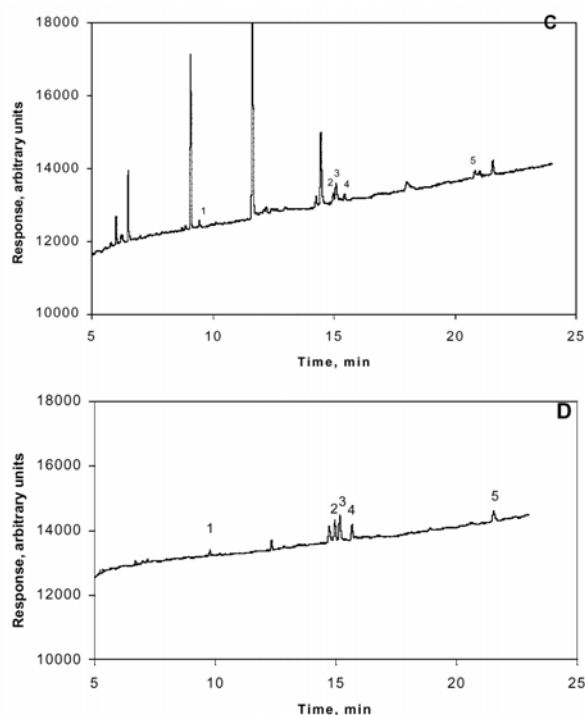
(T. Scharnweber)

1.3.2 Sol-Gel Glass Immunosorbent-Based Determination of s-Triazines in Water and Soil Samples Using GC/NPD

Funding: DAAD

Cooperation: Department of Botantics, TUM (PD Dr. K. Kramer, Prof. B. Hock)

Notwithstanding its prohibition in the European Union, especially atrazine is repeatedly detected in water bodies. There is a huge number of applications known to be used for monitoring triazine herbicides by LC and GC. Whatever system used, screening programs of pesticides require extraction, cleanup and preconcentration steps. Immunoaffinity chromatography (IAC) provides a selective method for sample preparation prior to LC and GC analyses. While the coupling of IAC with LC, in on-line or off-line mode, has been reported for several applications, less data are available in the literature concerning the combination of IAC and GC. Therefore, in this project we focused on the preparation of sol-gel glass immunoaffinity support using a monoclonal anti-atrazine antibody and its use for cleanup of surface water and soil extracts followed by the determination of s-triazines by GC/NPD. The cross-reactivity of the antibody for analytes structurally related with atrazine enabled the simultaneous extraction of several s-triazine herbicides (atrazine, propazine, terbuthylazine, cyanazine, deethylatrazine). After trace enrichment on the immunoextraction column, the s-triazines are desorbed by means of an acidic buffer and further extracted with ethylacetate before injected into the GC. Compared to liquid-liquid extraction (LLE) and solid-phase extraction (SPE) with a hydrophobic support, the GC-NPD chromatograms obtained after IAC of surface water (river water) samples or soil extracts and analysis, are free from matrix interferences. For example, non-specific adsorption of humic acids was not observed. The method allows the determination of the herbicides in linear ranges up to 1.5 $\mu\text{g/L}$ with correlation coefficients higher than 0.99 and relative standard deviations between 4 and 7% ($n = 5$). The LODs for 50-mL water samples are in the range 0.02 $\mu\text{g/L}$ (atrazine, propazine) to 0.1 $\mu\text{g/L}$ (deethylatrazine) ($S/N = 3$). In addition to its high selectivity, the immunosorbent proved to be re-usable for a significant number of preconcentration runs. (*C. Stalikas, University of Ioannina, Greece*)

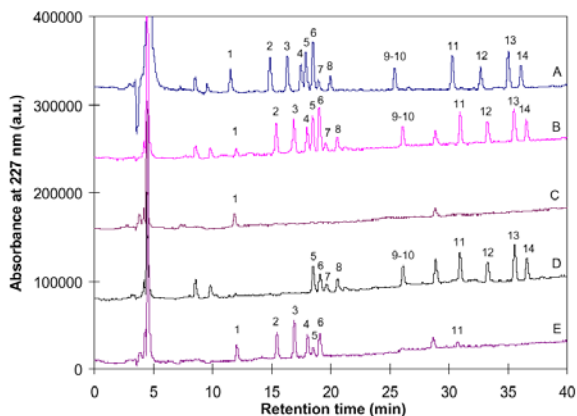


1.3.3 Preparation and Characterization of Molecular Imprinted Polymers (MIPs) for Sulfonylurea Herbicides

Funding: Alexander von Humboldt-Foundation

Sulfonylureas are potent herbicides, used in the control of broad-leafed weeds and some grasses in cereals. They are typically applied at rates of < 100 g/ha. These rates represent concentrations in environmental matrices of about 100 to 1000-fold less than other herbicides. Sensitive and reliable analytical methods are needed to evaluate their presence and persistence in water, soil and plant material at these very low levels.

Because of the low analyte concentrations, chromatographic techniques, including HPLC, need preliminary enrichment and cleanup steps. So far, solid-phase extraction using normal phase or reversed phase adsorbents and liquid-liquid extraction have been used for the cleanup.



Molecular imprinting is an increasingly applied technique which allows the formation of selective recognition sites in a stable polymer matrix. MIPs may be used as an artificial receptor to selectively bind the template (analyte) from a mixture of chemical species. In this project various MIPs are prepared, characterized (e.g. dissociation constant, binding specificity) and applied to enrich corresponding sulfonylureas from different environmental matrices. So far, the cleanup with the MIPs enabled a selective enrichment of 7 sulfonylureas in different water samples. Nicosulfuron, thifensulfuron-methyl, metsulfuron-methyl (MSM) and sulfometuron-methyl were recovered at 100% ($\pm 5\%$). Chlorsulfuron showed a recovery of 55% ($\pm 5\%$). Triasulfuron and prosulfuron can

also be enriched with the MIP, but showed only low recoveries (15-25%). MIPs proved to be very stable against organic solvents, high and low pH-values, pressure and temperature. The application to more complex matrices such as soil is ongoing.

(Q.-Z. Zhu, Xiamen University, China)

1.3.4 Determination of Sulfonylurea Herbicides Using Combined Immunoaffinity Extraction-Liquid Chromatography/MS/MS (IAC-LC/MS/MS)

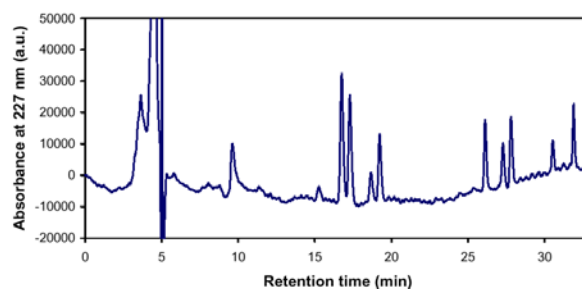
Funding: DFG Kn 348/8-1

Cooperation: Fraunhofer Institute of Molecular Biology and Applied Ecology (Schmallenberg)

Some reports have suggested that LC/MS/MS techniques do not require as much sample preparation or perhaps even none. Although the latter would be welcome to the analyst, practice is usually not that simple. Generally, the issues and strategies that have been important in sample preparation remain fundamentally important to reliable LC/MS/MS. A high degree of molecular selectivity can be achieved with affinity extractions, e.g. with immobilized antibodies (immunoaffinity extraction, immunoextraction, IE). Several supporting matrices have been chosen for the preparation of immunoadsorbents. Sol-gel technology which enables the incorporation of biomolecules into glasses has many advantages. So far, only few applications were reported in the literature using either polyclonal or monoclonal antibodies. Even less is the number of related papers, which describe the usage of sol-gel glass (SGG) immunoadsorbents for the enrichment of small analytes from real samples.

In the past, we have immobilized polyclonal antibodies against PAHs in SGG and applied for the selective extraction of these analytes from river and rain water, plant material and human urine. In this new project, several polyclonal and monoclonal antibodies will be prepared using haptens which comprise different structural parts of sulfonylurea herbicides. Then, the antibodies are encapsulated in SGG and the resulting immunoaffinity supports applied for the extraction of the herbicides from water and plant samples and subsequent determination by LC/MS/MS. Preliminary experiments with an existing polyclonal antiserum which was prepared against metsulfuron-methyl and used for combined RP18 SPE/SGG-IE cleanup allowed the enrichment of 8 sulfonylurea compounds from different spiked water samples (tap water, river water). The found recoveries were in correspondence with the cross-reactivity of the used antibodies. This method also showed an efficient removal of interfering matrix components.

(*P. Degelmann*)



1.4 Bioanalytics II

1.4.1 Development of a Biosensor for the Parallel Detection of Antibiotics in Milk

Funding: Forschungskreis der Ernährungsindustrie, FEI

Cooperation: LMU Munich (Prof. Märklbauer)

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, antibiotic-contaminated milk can result in the loss of cultured products (yoghurt and cheese) due to the inhibition of starter cultures and can cause significant economic damages.

For consumer protection, regulatory authorities have established residue limits (MRL) for several antibiotics in bovine milk (EC Regulation 2377/90). Microbial inhibition (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 β -lactam antibiotics before the milk is pumped out of the dairy van to avoid problems in the milk processing. Other antibiotic groups can not be determined with these tests. Furthermore, the dairy has to dispose the whole milk of a dairy van in case of a positive test result, which entails costs for the processing in a bioreactor and the deterioration of the value of the milk. To avoid the contamination of the collected milk, a sensor is necessary, which enables the rapid detection of all relevant antibiotics before the milk is pumped into the dairy van.



The basis for this sensor is the PASA system (Parallel Affinity Sensor Array) in which an indirect ELISA format is used on a biochip. Analyte molecules are immobilized as haptens in an array of spots on a biochip with a spot density of 4 spots/mm². The glass chip is silanized before, to obtain a hydrophobic surface on which hapten protein conjugates can adsorb. The spots are created by a non-contact spotting system with a piezo tip. The diameter of the spots is about 250 μ m. The disposable chip is integrated in a flow cell of about 100 μ L volume, where all incubations and reactions are carried out. A first incubation step with sample/antibody solution is followed by a second incubation with peroxidase labelled antibody. The signal is generated by a chemiluminescence reaction of the horseradish peroxidase with a luminol-based substrate. Emitted light is detected by a cooled and highly sensitive CCD camera. For each spot the intensity of the 9 most intensive pixels is evaluated. Each hapten is immobilized in 4-6 spot replicates. The active area of the biochip allows the integration of a large number of analytes, which is at the moment limited by the availability of suitable antibodies.

At present the parallel detection of the following analytes is possible in whole milk (detection limits and MRLs in brackets): streptomycin 0.5 μ g/L (200), cloxacillin 0.1 μ g/L (30), sulfadiazine 1 μ g/L (100) and sulfamethazine 0.9 μ g/L (100). All analytes can be detected far below the respective MRL. The test duration is 9 minutes, with potential for a further reduction. There is no sample preparation necessary. A reduction of the cycle time, the integration of further analytes as Penicillin G and Ampicillin and a covalent immobilisation of the haptens on the chip surface will be the next tasks.

(B. Knecht)

1.4.2 Development of Fast Immunological and LC-ESI-TOF-MS Methods for the Analysis of Cyanotoxins (Microcystins) in Drinking and Surface Water

Funding: BMBF 02WU9848/9

Cooperation: AWQC Adelaide, Australia (Prof. Bursill)

Cyanobacteria (also known as blue-green algae) are widely distributed microorganisms with occurrence in marine environment as well as freshwater. Some species produce toxins which are a hazard to human health when ingested with drinking water or during bathing in contaminated surface water.

The most frequently found cyanotoxins during freshwater blooms are the microcystins. Hepatotoxic cyclic heptapeptides (MW 800 - 1,100) contain two variable L-, three D-amino acids and two unusual amino acids, N-methyldehydroalanine and Adda ((2S,3S,8S,9S)-3-amino-9-methoxy-2,6,8-trimethyl-10-phenyldeca-4,6-dienoic acid). Adda is also found in the cyanotoxin nodularin – a closely related cyclic pentapeptide found in marine blooms.

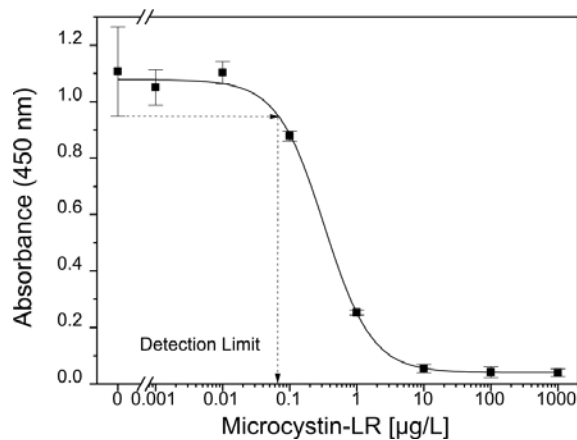
Microcystins and nodularin are highly toxic substances causing acute and chronic liver damage and intestine injury. Microcystin-LR and nodularin are also suspected to have tumor promoting activity. The World Health Organization (WHO) proposed a provisional guideline value of 1 $\mu\text{g/L}$ for the best known microcystin-LR in drinking water based on the tolerable daily intake (TDI, lifetime consumption) of 0.04 $\mu\text{g/kg}$ body weight for this toxin.

Only a few of the currently known toxic microcystin variants are commercially available. Therefore, the analysis of microcystins is still a considerable challenge. Analytical techniques with high sensitivity are needed, often incorporating enrichment, chromatographic separation and specific detection of the analytes such as mass spectrometry.

An enzyme-linked immunosorbent assay (ELISA) using antibodies with broad specificity provides an opportunity to measure the analytes without complicated enrichment and detection techniques. For this purpose a monoclonal antibody against the amino acid Adda, which is a part of all microcystins, was generated. It has a very broad recognition pattern for microcystins and nodularin. The established direct competitive ELISA calibrated against microcystin-LR shows midpoints below 1 $\mu\text{g/L}$ and detection limits below 0.2 $\mu\text{g/L}$ for all tested Adda-containing analytes. Also microcystin-LA which was discriminated by another microcystin-LR antibody has a detection limit of 0.056 $\mu\text{g/L}$. The new ELISA was applied for the measurement of surface water samples from Bavarian lakes and cyanobacteria containing algal food samples.

The monoclonal antibodies generated in this project can be applied for group-specific enrichment and detection of the toxins in liquid chromatography as well. A multidimensional biochemical detection of microcystins was shown using three antibodies and protein phosphatase 1 (PP1) as off-line detectors after HPLC separation of the toxins.

(I. Schaupt, A. Zeck)



1.4.3 Screening of Allergen-Specific IgE Using a Chip-Based System

Funding: Technical University of Munich

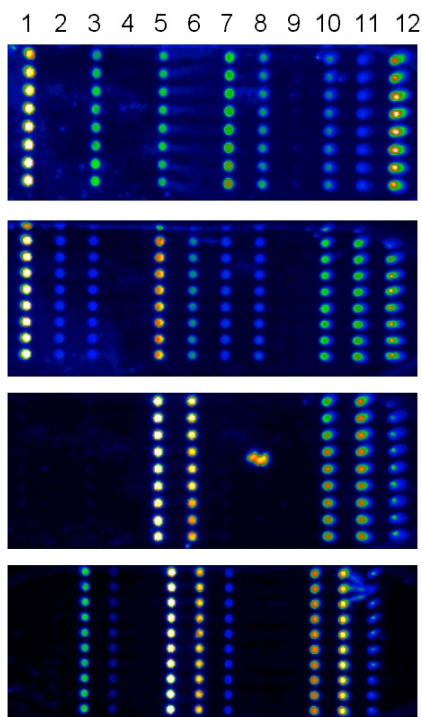
Cooperation: Department of Dermatology and Allergy, TUM (Prof. J. Ring)

An increasing number of patients are suffering from allergies such as hay fever, asthma or food allergies. Since 1967, when the radio-allergo-sorbent assay (RAST) for serum immunoglobulin E (IgE) and allergen-specific antibodies in serum was described, many various assay procedures have been developed, but only a few have become routine methods in clinical chemistry, immunologic laboratories or in doctor's offices.

Many of these assays are based on ELISA techniques. Although it is possible to measure 96 samples with one microtiter plate, a complete determination of the allergen-specific IgE level in the patients' blood is expensive and time-consuming. In addition, to measure n allergen-specific IgE antibodies the n -fold volume of blood sample is needed. Although mixtures of different allergens in one assay can be used, the single components have to be broken down after a positive test result. Therefore, it is important to develop a fast and cheap screening technology for the allergen-specific IgE antibodies in blood samples.

We use glycidylxypropyl-modified glass slides as test platform. Self-made allergen extracts and recombinant/purified allergenic proteins were immobilized as small droplets (5 nL, spot diameter about 200 μm) on the chip platform using piezoelectric nanoliter pumps. Incubation with serum samples (200 μL 1:10 diluted sample, 30 min) and HRP-labeled anti-human IgE (1:500, 30 min) could be performed using chamber slides in combination with cover slips or with the flow cell of the PASA system. In the last step the chamber of the flow cell is filled with a chemiluminescence substrate reacting with bound HRP molecules under emission of light. The light emission is visualized with a CCD camera. If the serum sample contains antibodies against a special allergenic protein, light emission occurs at the position of the relevant allergic protein.

(B. Fall)



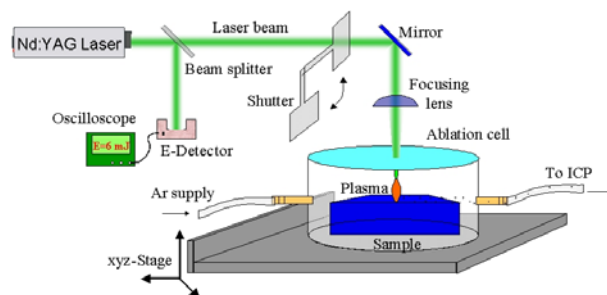
1.5 Laser Spectroscopy I

1.5.1 Analysis of Solid Samples by Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS)

Funding: IWC TUM

Elemental characterization of solids is one of the most important issues of inorganic analysis. In this field, laser ablation sampling can be an attractive alternative to common ICP-MS, where solution nebulization is used. The most important advantage of the technique is the avoidance of digestion procedures, saving much time and effort. Instead, a pulsed laser is focused on the surface of the sample, where it ablates a small amount of matter. The resulting aerosol is efficiently transferred to the ICP-MS, where the particles are atomized in an argon plasma at temperatures of about 8000 K. Analysis is performed by separation and quantification of the different ions within the plasma.

The aim of the project was to develop laser ablation methods for solid samples that are difficult to digest. An ablation system was designed and attached to a commercially available ICP-MS instrument. It consisted of a Nd:YAG laser and a motorized *xyz*-translation stage, on which the ablation cell was mounted. The sample was placed inside the cell and was accessed by the laser through a quartz window on top. The laser was operated either at the fundamental wavelength ($\lambda=1064$ nm) or at the fourth harmonic ($\lambda=266$ nm). The pulse energy was monitored via a beam splitter with a pyroelectric probe.



In the first part of the project, strategies were developed for representative analysis of solid samples with different grades of heterogeneity. The procedures were tested with binary mixtures of KNO_3 and SiO_2 particles of different sizes and concentrations. Thus, the theorem of Gy could be verified, which states that the critical sampled mass should contain at least 30 analyte elements. The findings were then applied for composition analysis of two classes of real samples: coals and automotive catalysts. Differences in ablation behaviour of various coals were corrected by addition of a binder or by standardization on intrinsic or extrinsic standards. Also, chemometric methods were applied. In this way, an accurate characterization was achieved for all samples.

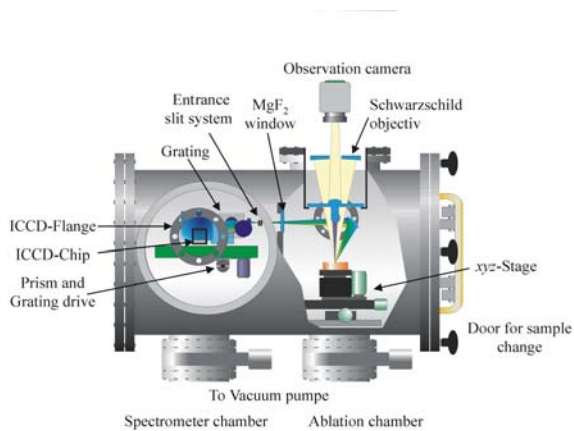
(H. Fink, L. Kleiber)

1.5.2 Microanalysis Using the Laser-Induced Plasma Spectroscopy (LIPS) and VUV-Echelle Spectrograph

Funding: DFG Pa 716/2-1

Cooperation: ISAS, Berlin

Aim of the project is the application of laser-induced plasma spectroscopy (LIPS) for quantitative spatially- and depth-resolved microanalysis using a new-designed VUV-Echelle Spectrograph. For that purpose, a high-intensity pulsed beam from a Nd:YAG laser is focused on the sample surface. A small amount of matter from the sample is ablated, vaporized and transformed in a localized plasma. After approximately one microsecond the characteristic radiation from the plasma, due to relaxation of excited atoms and ions, can be detected and used for the identification and determination of the elements in the sample.



Micro-LIPS system with VUV Echelle-Spectrograph

Applying the appropriate modification of the beam (“micro focusing”) LIPS allows fast spatially resolved elemental characterization of surfaces with a typical resolution of $10\ \mu\text{m}$.

Using the UV laser beam ($\lambda=266\ \text{nm}$) fractionization effects can be minimized and quantitative analysis can be performed. Analysis of the spectra from the single pulse LIPS allows a depth-resolved investigation of the sample in combination with a spatially resolved one.

Development of a high resolution ($\lambda/\Delta\lambda > 10000$) Echelle-spectrograph for the range between 150-300 nm makes, for the first time, a LIPS analysis of non-metals (S, P, N, O, As) and some metals (Hg, Zn) possible.

First applications are devoted to geological samples with highly irregular distribution of certain elements.

(I. Radivojevic)

1.5.3 Investigation of Biofouling by X-ray Microscopy and Asymmetric Field Flow Fractionation

Funding: BMBF 02WU9893/0

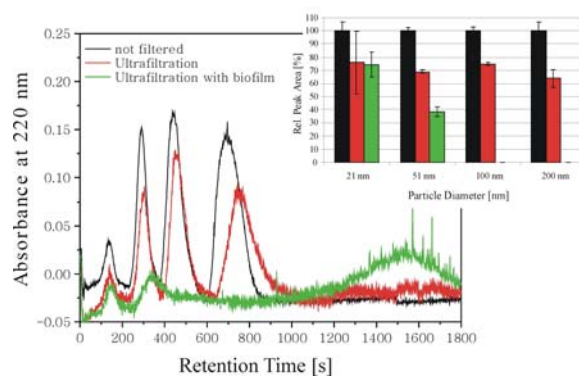
Cooperation: Institute for X-Ray Physics, University of Göttingen

The modification of the flow characteristics of a filter resp. filter clogging due to a growing biofilm is usually termed biofouling. The effect of biofouling appears as unwanted side effect in all systems for water treatment and purification. The aim of the investigations is the characterization of the ad-hoc status of a filter membrane. The study is based on the combination of X-ray microscopy (setup at the BESSY II via a collaboration with the University of Göttingen) and characterization of the filter via asymmetric field-flow fractionation (AF⁴).

A sample of a defined concentration, which consists of a mixture of PS-latex colloids is filtered with a polycarbonate membrane, serving as a model system, by applying overpressure. Then, the modifications of the filter pore can be examined with the transmission X-ray microscope or with the scanning transmission X-ray microscope (both located at BESSY II). X-ray microscopy allows a high spatial resolution and the ability to study colloidal structured directly in aqueous media. The penetration of the soft X-rays is sufficient to penetrate cells with a thickness of some micrometers. In a scanning transmission X-ray microscope the polychromatic synchrotron radiation is first reduced in its bandwidth by a grating monochromator. A micro zone plate focuses this radiation into a small focal spot within the sample. By moving the zone plate over the object and recording the transmitted signal an image of the sample can be generated.

Our studies concentrated on the analysis of the colloidal transmission during biofilm growth by asymmetric field flow fractionation. AF⁴ is an analytic separation technique for fractionation and size determination of particles and polymers. Particles between 1 nm and 100 μm, as well as polymers between 1000 and 10⁶ Da can be addressed. The advantages are the small expenditure for the sample preparation, the gentle separation conditions, and the possibility of pre-concentrating diluted samples in the separation channel. The separation takes place in a channel of approximately 300 mm length, 250 μm height, and 10 mm breadth. In general, FFF exploits the simultaneous action of a carrier flow and an external field, which induces a differential migration on unlike particles inside the separation channel. In the case of AF⁴, a cross flow is directed at a right angle to the laminar carrier flow as an external field. The external field drives the particles against the accumulation wall. Dependent on the diffusion coefficient, a net re-diffusion takes place. Hence, the separation is caused by interaction between a concentration gradient and parabolic flow velocity profile. Thus, in the normal separation mode smaller particles elute earlier than the large particles. The experiments demonstrated that the AF⁴ can be utilized to detect and quantify modifications of the filtration characteristics of PS colloids after biofilm growth. Further, we could show the biofilm growth does not lead to a uniform modification of the filter but preferential retention of some particles sizes.

(*S. Hegendorf*)



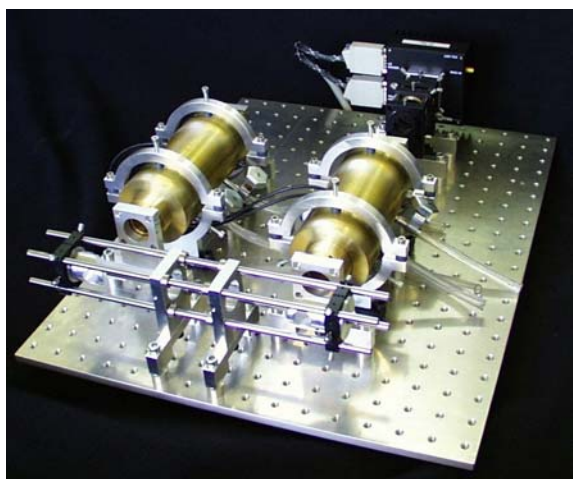
1.6 Laser Spectroscopy II

1.6.1 Development of a Photoacoustic Sensor System for Time-resolved Soot Measurement in Diesel Exhaust

Funding: VFI, Frankfurt

Motor vehicles like cars and heavy duty trucks are major sources of air pollution. Particulate mass emitted by diesel engines consists mostly of carbonaceous material. The influence of soot particles on human health as well as global and local climate is well established by now and led to recent regulations demanding a reduction of particle emission in diesel exhaust up to 90 % within the next years. This is not only a challenging task for car manufacturers to design a new generation of low emitting engines and new particle filter systems, it also brings the classical analytic methods to their limits.

The measurement of elemental and organic carbon is conventionally accomplished by particle collection on filters, followed by thermochemical or thermogravimetric detection methods. Wet chemical analysis and combustion require well equipped laboratories and time consuming sample preparation. Due to the integration on a filter, a time-resolved analysis is not possible. To meet the new emission regulations a new generation of measurement instruments for process monitoring are needed. Requirements for such systems are high sensitivity combined with high selectivity for elemental carbon. Their implementation will be only possible if time-resolved soot detection with sufficient sensitivity can be realised.



The highest particle emissions from diesel engines are generated during load changes. Within such load changes the emitted soot concentrations can rise several orders of magnitude for a period of few seconds to decrease immediately afterwards. Process studies afford a fast time response with a sampling rate in the range of 1 Hz. Mobile systems with a certain simplicity and economic efficiency are generally preferred. The presented photoacoustic sensor system is optimised for a highly sensitive and fast on-line and in situ quantification of soot.

The system combines a time resolution of 1 s (sampling rate 3 Hz) with an aerosol mass sensitivity better than $10 \mu\text{g}/\text{m}^3$. The system consists of two photoacoustic cells, which are operated in a differential mode to avoid cross sensitivities to any molecular absorption. The cells were built as acoustical resonators to increase sensitivity. A diode laser with a wavelength of $>810 \text{ nm}$ and an output power of $>1 \text{ W}$ was employed for excitation. To avoid condensation of water, the cells are heated to 50°C . The whole system is incorporated into a 19"-rack.

The design is rugged for field applications at an engine test site to withstand external acoustic noise, temperature fluctuations, and dust contamination. The overall performance and figures of merit were established under laboratory conditions with soot aerosols generated by a spark discharge aerosol generator. Meanwhile, the system is routinely used for engine development at engine test sites. At the site, the system was calibrated by recording several stationary cycles. The time resolution was validated by on-line measurements of transient cycles. Throughout all experiments, reference analysis was performed via a thermochemical standard procedure, i.e. a German

standard reference method (VDI guideline 2465, sheet 1).

(H. Beck)

1.6.2 Fast Measurement of Soot Immission by Photoacoustic Spectroscopy

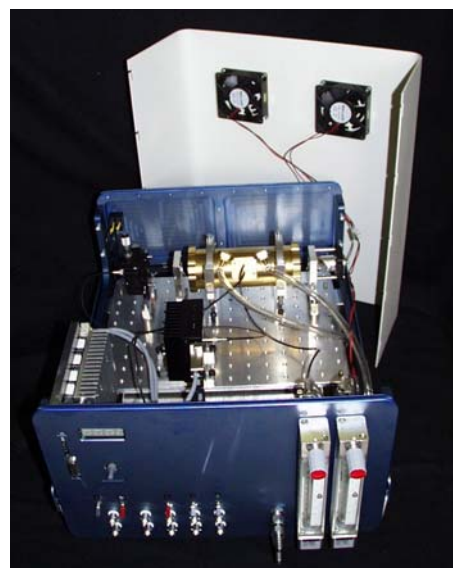
Funding: BayStMLU within project SCAVEX

Due to their size soot particles can easily be incorporated through respiratory organs. Their chemical and physical properties make them a potential risk for human health. As classical "black absorber" soot absorbs electromagnetic radiation over the whole spectrum and therefore acts as greenhouse gas influencing the global climate. Soot also has an important role in cloud nucleation processes and thus can influence the local climate as well. Hence, the need for a fast and sensitive soot detection in urban and remote areas is obvious. The state of the art thermochemical detection methods for soot analysis are based on filter sampling and subsequent wet chemical analysis and combustion, which require laborious and time consuming sample preparation. Due to the accumulation on a filter, time-resolved analysis is not possible and the extensive sample preparation cause long delays between sampling and measurement result.

The photoacoustic spectroscopy enables a highly selective and sensitive detection of soot without sample preparation in a short time interval. Therefore the analyte is excited by a modulated laser beam. The energy absorbed by the particles is converted into heat by non-radiative relaxation processes. According to the gas law the emitted heat is transformed into pressure fluctuation which can be detected by pressure sensitive detectors like microphones. The presented system was designed to detect very low concentrations of soot ($<1 \mu\text{g}/\text{m}^3$) with a moderate time resolution in the minute range. It is meant for atmospheric soot detection in remote areas and high altitude, which are supposed to reveal background concentrations of soot without direct contamination by traffic and industry.

The system consists of a single cell containing a longitudinal acoustic resonator. The aerosol stream is divided into two branches. One of these branches is sucked through an absolute filter in order to get air without particulate matter. Differential measurement procedure can be performed by switching between these branches with the help of a magnetic valve. The properties of the cell were determined by water vapour absorption measurements using an external cavity diode laser at 6930 /cm . The sensor system was characterised under laboratory conditions with model soot generated by a spark discharge generator (PALAS, GFG 100). Measurement control and signal processing were performed by a computer program written in LabView. One single test cycle takes approximately 5 minutes and includes the measurement of the analyte and the background signal. This system was developed to be a stand-alone measuring instrument working without need of system regulation after it has been started. Due to this requirement data transfer and status information reports can be transmitted via modem over far distances. At present this system is installed in an observatory on top of Mount Zugspitze (2964 m).

(H. Beck)



1.6.3 On-line Measurement of Highly Concentrated Dye Solutions by Photoacoustic Spectroscopy

Funding: IWC TUM

The colouring of textiles is performed with high concentrated dye solutions. The dyeing process and thus the dilution of the solution is usually controlled visually without any technical instruments. To achieve a constant quality level, an automated monitoring of various process steps, e.g. the dye concentration of the bath, is of great significance. Conventionally, concentration measurements of coloured solutions can be performed by transmission spectroscopic methods according to the Lambert-Beer law. Due to saturation effects transmission spectroscopy is only linear in a small concentration range. Furthermore it is severely influenced by light scattering particles. To measure highly concentrated and strong absorbing samples like dye solutions these techniques require a great deal of sample preparation.



Photoacoustic spectroscopy (PAS) is a promising technique to fulfil all requirements for such an application. When light is absorbed by a sample, a part of the absorbed energy is converted into heat, respectively pressure. This phenomenon is called "photoacoustic effect". Since only absorbed energy can be converted into heat, PAS is free of interference by light scattering particles. Selectivity is obtained by selection of the excitation wavelength. The signal amplitude is proportional to the optical absorption coefficient and the concentration of the analyte. After calibration of the system, on-line quantification is possible. Linearity is achieved for a wide range, therefore dye concentrations can be determined over several orders of magnitude.

The prototype of an on-line measurement system was developed within the framework of this project. A dye laser pumped with an excimer laser was used as light source at the wavelengths of 550 nm and 650 nm with an optical energy of 200 μJ per pulse. The laser beam was focused into the flowcell. The acoustic pulse is detected with a piezoelectric sensor on the opposite of the irradiated site. For this application, three different sensor heads were developed. They are based either on PZT ceramics, PVDF foils or electromechanical foils. The piezoelectric material is connected to the sample by an acoustic coupling layer. The electronic signals were amplified by a preamplifier and analysed by a digital oscilloscope. Data processing was performed with a standard computer.

In a first set of experiments the quantification of textile dye concentration from 100 mg/L up to 25 g/L was performed without sample preparation. The signal was not influenced by the flow through the cell. Further experiments will focus on the influence of light scattering particles at different concentrations. Signal dependence by the temperature will also be studied, as well as mixtures of different dye solutions, that can be measured by the use of more laser wavelengths.

(C. Helmbrecht)

1.6.4 Biofilm Monitoring by Photoacoustic Spectroscopy (PAS)

Funding: DFG Ni 261/14-1

Biofilms are aggregates of microorganisms which occur at aqueous interfaces. Biofilms attached to solid surfaces can be found in natural and engineered water systems. The unwanted deposition of biofilms in technical processes is termed biofouling. Biofouling

in technical processes reduces the water quality and increases the frictional resistance in tubes. In wastewater treatment plants, biofilms are used for removal of organic pollutants. For improvement of anti-fouling strategies and for process optimization in wastewater treatment plants, an analytical technique for on-line monitoring of biofilms is needed.

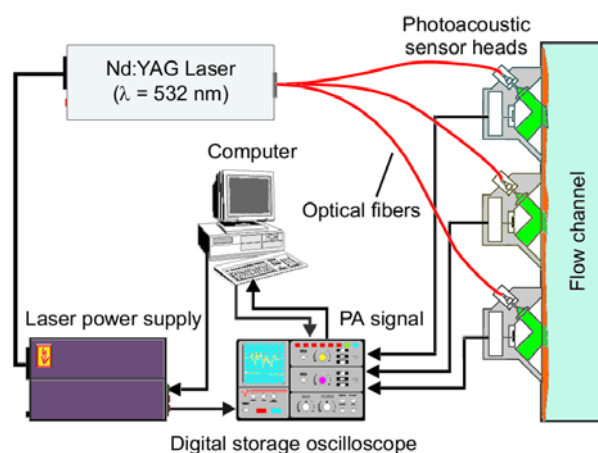
Within the presented project, photoacoustic spectroscopy (PAS) is used as a new biofilm monitoring technique. The photoacoustic sensor heads consisted of a 25 μm thick wide-band piezoelectric poly(vinylidene)difluoride (PVDF) film which was coupled to a transparent prism by a conductive epoxy. The piezoelectric film was integrated into a BNC socket to eliminate electromagnetic interference. The sample was irradiated through one side and the base of the prism. In this way, an indirect detection scheme has been realized, i.e. excitation and detection of pressure waves are performed from the same side of the sample.

The characterization of the sensor heads was performed with biofilm models consisting of agar-agar hydrogels. The sensor system allows the depth-resolved analysis of aqueous samples (aqueous solutions, hydrogels and biological tissues) with a depth resolution of about 10 μm and a detection limit for the absorption coefficient of 0.02 /cm at a laser pulse energy of $E_0 = 1 \text{ mJ}$.

Experiments with biofilms growing directly on the sensor heads demonstrated the potential of PAS in the field of biofilm monitoring. Photoacoustic spectroscopy allows nondestructive investigation of biofilms. By photoacoustic absorption measurements in the visible spectral range (Nd:YAG laser at $\lambda = 532 \text{ nm}$), growth and detachment of biofilms which were associated with the sensor surface could be monitored. Important changes in the biofilm due to changes in pH-value, flow conditions, particulates etc. could be detected for the first time in a depth-resolved fashion by photoacoustic measurements at three different positions inside a flow channel.

Within further investigations, a tunable laser system is used for excitation of photoacoustic signals. An optical parametric oscillator which is pumped by a Nd:YAG laser allows the generation of short laser pulses in the wavelength range from 410 nm to 2550 nm. With this system photoacoustic absorption spectra of biofilms will be measured and thus, changes in the composition of the biofilm will be monitored.

(T. Schmid)

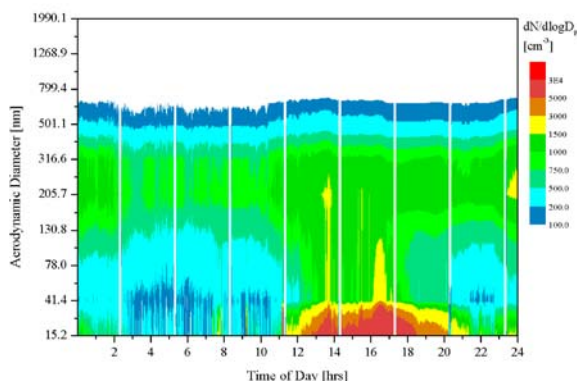


1.7 Aerosol Research

1.7.1 Schneefernerhaus Aerosol and Reactive Nitrogen Experiment (SCAVEX)

Funding: BayStMLU

To allow an accurate assessment of the influence of aerosols on atmospheric chemistry and climate, a thorough physical and chemical analysis of atmospheric aerosols is required, including the characterisation and quantification of organic particle components. The SCAVEX aerosol measurement program at the Schneefernerhaus observatory (UFS) is aimed at an extensive physical and chemical characterisation of air particulate matter in the high alpine environment, where either boundary layer air or free tropospheric air prevail under different meteorological conditions. It is carried out by the Technical University of Munich (Institute of Hydrochemistry), the Vienna University of Technology (Institute of Analytical Chemistry), the Paul Scherrer Institute (Atmospheric Chemistry Laboratory), and the University of Clermont Ferrand (Institute of Physical Meteorology) in collaboration with the German Aerospace Center (DLR, Institute of Atmospheric Physics) and the German Weather Service (DWD). Within SCAVEX the aerosol measurements at UFS are complemented by trace gas measurements (DLR and its partner MPIK Heidelberg), and during intensive campaigns also by airborne measurements of both particles and gases onboard the DLR research aircraft Falcon (DLR and MPIK Heidelberg). Meteorological data are provided by the DWD and by the DLR partner KNMI. The University of Munich (Institute of Statistics) contributes statistical analyses of the combined aerosol, trace gas and meteorological data.



During 2001 several measurement campaigns and some long-term measurements have been performed at the Schneefernerhaus observatory with the following instrumentation: A condensation particle counter for particle number concentration monitoring, a differential mobility particle sizer (DMPS) and an electrical low pressure impactor (ELPI) for particle size distribution measurements, and several filter samplers (Hi-Vol, Lo-Vol, PM2.5). Also a photoacoustic soot sensor and a multi-wavelength aethalometer have been applied. A CN-sampler for water vapor condensation nuclei is under construction and will be deployed in future campaigns. Analytical techniques for various classes of organic particle components, in particular for polycyclic aromatic compounds and biopolymers have been developed, and some of them have already been applied to the collected filter samples. In the future also the particulate matter deposited on the ELPI impaction substrates will be subject to chemical analysis.

Depending on the meteorological situation, the observed total particle number concentrations varied typically from a few hundred up to a few thousand particles per cubic centimetre. At low particle concentrations, i.e. under clean conditions such as free tropospheric air, the number size distributions exhibited a maximum in the accumulation mode (particle diameter: ≈ 100 nm). At high particle concentrations different size distribution patterns were observed, on some occasions a strong nucleation mode (particle diameter: ≈ 20 nm) dominated the total number concentration, in others also the accumulation mode was enhanced. An example for a nucleation mode event is shown in the figure (measurement date: 01.05.2001).

(*S. Kamm, K. Krause, A. Messerer, A. Zerrath*)

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

Funding: BMBF AFO 2000 07ATC05

The influence of aerosols on atmospheric chemistry and physics, climate and human health is one of the central topics in today's environmental research. Besides the aerosol particles' size distribution their chemical composition is the primary parameter governing heterogeneous and multiphase chemical reactions in the atmosphere, formation of clouds and precipitation, radiative climate forcing effects, and health effects of aerosols.

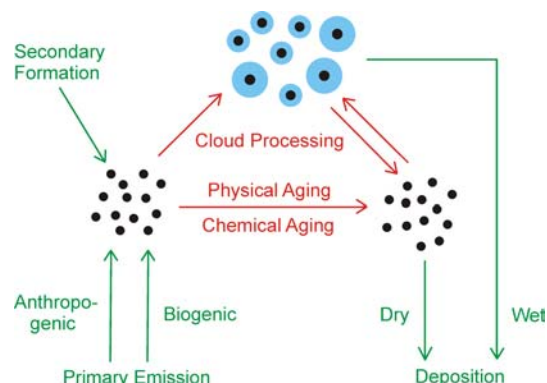
Several studies have shown that carbonaceous components are major constituents of tropospheric aerosols (10-50% mass fraction), that black carbon is the main light absorber in air particulate matter, and that organics can strongly affect the physicochemical particle properties. The actual composition of atmospheric particles is, however, spatially and temporally highly variable, and in particular carbonaceous components have been characterized only sparsely and incompletely up to now.

Therefore the central aim of the CARBAERO project is to characterize the molecular structures and abundances, reactivity and hygroscopicity of carbonaceous aerosol components. The investigations are focused primarily on aromatic compounds, macromolecules (biopolymers and humic-like substances), and elemental carbon, and the following key questions are addressed:

- How is the composition of carbonaceous aerosol components changed by chemical aging (reaction products and kinetics), and how can these processes be efficiently described in atmospheric models?
- What are the effects of carbonaceous aerosol components and their aging on the interaction of atmospheric particles with water vapour, on the activation of cloud condensation nuclei, and thus on the indirect radiative effect of aerosols on climate?
- Can the chemical aging of carbonaceous aerosol components affect the optical properties of atmospheric particles and thus influence the direct radiative effect of aerosols on climate?
- Which characteristic features or tracers are best suited to attribute carbonaceous aerosol components to different natural and anthropogenic sources (combustion processes, suspension of biological material, etc.)?

In the year 2001 research activities have been pursued and scientific results have been achieved in the following areas:

- Development and optimization of analytical methods for the determination of polycyclic aromatic compounds, carbohydrates and proteins in atmospheric aerosol samples (extraction schemes, chromatographic and spectrometric methods, enzymatic assays).
- Field measurement campaigns at urban and suburban sites in Munich and at the high alpine GAW observatory Schneefernerhaus on Mount Zugspitze: (aerosol particle number concentration and size distribution measurements, gravimetric and chemical analysis of filter samples): characteristic differences in the physical properties (particle number/mass concentration and size distribution) and chemical composition (TC/EC, WSOC, PAHs, proteins).



- Aerosol flow tube investigations of the interaction of spark-discharge soot particles (with/without PAH-coating) with reactive trace gases (O_3 , NO_2) and water vapor: kinetic and mechanistic description of competitive adsorption and surface reaction processes.
- Investigation of the hygroscopic growth of aerosol particles with complex chemical composition (HTDMA- experiments with mixtures of biopolymers, salts, etc.)

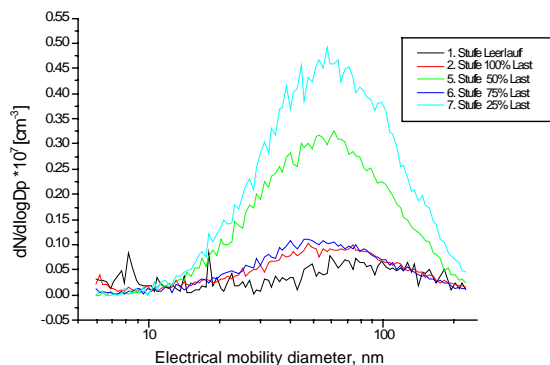
(M. Elsässer, T. Franze, S. Kamm, K. Krause, C. Schauer, A. Zerrath)

1.7.3 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, Garmisch-Partenkirchen; Fritz-Haber-Institute, Department of Inorganic Chemistry, Berlin; Max-Planck-Institute for Polymer Research, Mainz.

The research activities at IWC are focused on the development and characterisation of filterless soot particle deposition traps and on the kinetic investigation of the oxidation of deposited soot particles.



The new catalytic structures to be developed in this project will circumvent the problems of conventional soot filters (increased fuel consumption due to increased exhaust pressure, uncontrolled soot burn on the filter, blocking and necessity for regeneration) by applying so called open-structures, which are developed in cooperation with Oberland-Mangold. Phoretic effects in addition to the other involved particle deposition processes (interception, impaction, diffusion, sedimentation and electrostatic precipitation) will be investigated in detail with a specially designed plate precipitator.

The deposition performance of the investigated catalyst structures will be examined at the model exhaust gas test bench with a newly designed flat-bed-reactor, which can be loaded with model catalyst structures and applied to soot-laden model exhaust gas. The deposition performance will be investigated with Differential Mobility Analyzers and condensation particle counters.

At MAN the physical properties of diesel exhaust particles from different engine types at varying sample positions is investigated with different dilution systems and differential mobility particle sizing system. Additionally, the chemical composition of soot particles from EURO IV/V is investigated with a wide variety of analytical techniques.

The second part of the investigations at the IWC focuses on the characterisation of the heterogeneous soot oxidation processes occurring in the particle traps in presence of NO_2 . The exact kinetics of the participating reactions are not fully known in detail up to now. Moreover the influence of catalytic coatings (Metal oxides for the oxidation of NO as well as soot) will be investigated. Kinetics experiments will be performed with spark discharge soot, high-molecular weight polycyclic aromatic hydrocarbons synthesized at the MPI in Mainz, and real diesel soot.

(D. Rothe, A. Messerer)

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2.2 Conference Presentations

2.2.1 Oral Presentations

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- H. Beck, C. Haisch, R. Nießner: Development of a Photoacoustic System for Fast Measurement of Black Carbon Particles, 5th Euroconference on Environmental Analytical Chemistry, 8.-12.9.2001, Blarney, Ireland.
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- T. Baumann & C. J. Werth, Visualization of Colloid Transport Using Magnetic Resonance Imaging, AGU Fall Meeting, 10.-14.12.2001, San Francisco.
- T. Baumann & R. Niessner, Assessment of the Pore Space Topology From Colloid Filtration, AGU Spring Meeting, 29.5.-2.6.2001, Boston.
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- D. Rothe, S. Kamm, H. Baumann, E. Jacob, R. Nießner, U. Pöschl, Bestimmung des Sulfatgehalts von Dieselabgaspartikeln, ANAKON 2001, Konstanz, 4.4.-7.4.2001.
- T. Scharnweber, D. Knopp, R. Nießner: Charakterisierung eines monoklonalen Antikörpers gegen Benzo[a]pyren und Entwicklung eines Enzym-Immunoassays (ELISA). Jahrestagung 2001 der Wasserchemischen Gesellschaft in der GDCh, Bad Wildungen, 21.-23.05.2001
- C. Schauer, T. Letzel, R. Nießner, U. Pöschl: Analysis of Polycyclic Aromatic Aerosol Components. European Aerosol Conference 2001, Leipzig, 3.-7.09.2001D 300

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- M. Seiss, R. Nießner: Neue Strategien zur Überwachung geschlossener UV-Reaktor-Geometrien. Jahrestagung 2001 der Wasserchemischen Gesellschaft in der GDCh, Bad Wildungen, 21.-23.05.2001
- C. Vogt, N. Nestle, F. Stallmach: NMR-Untersuchungen an Aquifermaterialien. Jahrestagung 2001 der Wasserchemischen Gesellschaft in der GDCh, Bad Wildungen, 21.-23.05.2001
- A. Zerrath, R. Nießner, U. Pöschl, Untersuchung des Kohlenhydratgehalts atmosphärischer Aerosolproben, ANAKON 2001, Konstanz, 4.4.-7.4.2001.
- Q.-Z. Zhu, P.B. Carrasco, S.G. Sire, K. Haupt, M. Schedl, T. Scharnweber, J.M. Bayona, D. Knopp, R. Niessner: Die Herstellung molekular geprägter Polymere (MIPs) für Sulfonylharnstoff-Herbizide am Beispiel von Metsulfuron-methyl. ANAKON 2001, 4.-7. 4. 2001, Konstanz.

2.2.3 Invited Lectures

- T. Baumann, Sketches for synchrotron radiation experiments for hydrogeology and aerosol chemistry, ANKA Synchrotron Environmental Laboratory, 1st Users Meeting, 29.-30.3.2001, Karlsruhe.
- D. Knopp, Analytical application of immunoassays: Determination of polycyclic aromatic hydrocarbons (PAHs) in water, soil, air and human body fluids. 2nd International Conference on Instrumental Methods of Analysis, Modern Trends and Applications, 5.-8. 9. 2001, Ioannina, Greece.
- D. Knopp, Class on Development and Application of Modern Bioanalytical Methods, Department of Analytical Chemistry, Faculty of Sciences, University of Pècs, 24.-29. 9. 2001, Pècs, Hungary.
- N. Nestle, NMR-Techniken zur Beobachtung der Hydratations-Kinetik und der Wasserdynamik in Zement, Schlacke und verwandten Materialien, 8.6.2001, Ludwig-Maximilians-Universität München, Mineralogie.
- N. Nestle, Zement - ein alltäglicher Baustoff als aktueller Forschungsgegenstand der Physik und Chemie, Anregungen für einen fachübergreifenden Unterricht, 3.7.01, Universität Erlangen, Physikdidaktisches Kolloquium.
- N. Nestle, NMR-Methoden zur Untersuchung härtender mineralischer Bindermaterialien, 16.7.01, Fraunhofer-Inst. für zerstörungsfreie Werkstoffprüfung, Saarbrücken.
- N. Nestle, Zement - ein harter Brocken weicher Materie, 20.9.01, Physikalisches Kolloquium der BASF, Ludwigshafen.
- N. Nestle, NMR-Messungen zur zerstörungsfreien Beobachtung der Strukturbildung in hydratisierendem Zement und verwandten Materialien, 23.10.01, Universität Leipzig, Mineralogisches Kolloquium.
- N. Nestle, NMR-Messungen an Geo- und Umweltmaterialien, Stand und Perspektiven, 29.11.01, Universität Jena, Forum Angewandte Geologie.
- R. Nießner, Aktuelle Probleme des Wasserkreislaufes und Analytische Chemie. Universität Dortmund, GDCh-Vortrag, 15.01.2001, Dortmund.
- R. Nießner, Lasergestützte Spektroskopie an Umweltmatrices ohne Massenspektrometrie. 34. DGMS-Diskussionstagung, 4.-7.03.2001, München.
- R. Nießner, Analytische Charakterisierung von Verbrennungsaerosolen. Mitarbeiterseminar des Fachgebietes Chemische Analytik, 27.04.2001, TH Darmstadt.

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- R. Nießner, New Analytical Techniques within Water Treatment Processes. Special Joint Chemical Engineering, Chemistry, and IGERT Seminar, 2.05.2001, Lexington, USA.
- R. Nießner, New Trends and Needs for Chemical Field Screening. 2nd Int. Conf. Field Screening Europe 2001, 14.-16.05.2001, Karlsruhe.
- R. Nießner, What is Air Pollution? Euroconference "Chronic Lung Disease", Institut Pasteur, 27.06.2001, Paris.
- R. Nießner, Neue Aufgaben für die Wasseranalytik am Beispiel der Anforderungen aus der EU-Direktive (Trinkwasser) sowie zur Microcystin-Problematik. VBGW-Fachtagung WASSER 2001, 28.06.2001, Bad Reichenhall.
- R. Nießner, Laser-based Photoacoustic Spectroscopy for Environmental Monitoring. IUPAC International Congress on Analytical Sciences 2001, 6.-10.08.2001, Tokio.
- R. Nießner, Analytical Characterization of Sensitive Parameters Within the Hydrologic Cycle. Int. Conf. IMA 2001, 5.9.2001, Ioannina.
- R. Nießner, Analytische Methoden der Aerosol-Quellenerkennung. Workshop "PM_x-Quellenidentifizierung": Möglichkeiten und Ergebnisse, 12.9.2001, Duisburg.
- R. Nießner, Immunserological Detection of Harmful Substances within Water, Air and Soil. ExTech 2001, 18.9.2001, Barcelona.
- R. Nießner, Charakterisierung von Wasserinhaltsstoffen mittels optothermischer Laserspektroskopie. GDCh-Hauptversammlung, 24.9.2001, Würzburg.
- R. Nießner, Neue Meßaufgaben und Verfahren für die Sensorik in der Wasserchemie. 5. Dresdner Sensor-Symposium, 10.12.2001, Dresden.
- U. Panne, Trends in Analytical Laser Spectroscopy, CANAS '01, 11.-15.3.2001, Freiberg.
- U. Panne, 'More Lasers, More Fun - Spektrochemische Analyse mit Lasern', GDCh-Vortrag, 4.12.2001, Universität Kassel.
- U. Pöschl, Formation and Decomposition of Carcinogenic, Mutagenic and Allergenic Aerosol Particle Components, 13th Congress of the International Society for Aerosols in Medicine (ISAM), Interlaken, 17.9.2001.
- U. Pöschl, Aerosolpartikel und Kohlenstoff in der Atmosphäre, TELI Journalistenvereinigung für technisch-wissenschaftliche Publizistik, München, 25.9.2001.
- M. G. Weller, Vom Immunoassay zum Biochip, 15.1.2001, Institut für Chemie und Biochemie der Universität Greifswald.
- M. G. Weller, Difficulties on the Way to a Glufosinate Immunoassay, 23.4.2001, Artefacta II, Basel, Schweiz.
- M. G. Weller, Moderne immunologische Methoden in der Spurenanalytik, 13.7.2001, CEAC Sommer-Workshop 2001, EAWAG/EMPA-Akademie Dübendorf, Schweiz.
- M. G. Weller, ESI-orthogonal-TOF-MS zur Identifizierung von cyanobakteriellen Toxinen in Oberflächengewässern, 27.9.2001, GDCh-Jahrestagung Chemie, Würzburg.
- M. G. Weller, Immunchromatographische Kopplung - eine interessante Methode zur Erhöhung der Spezifität, 14.11.2001, HPLC-Tage 2001, Mannheim.
- M. G. Weller, Bioaerosole - Analytik einer neuen Dimension (Habilitationvortrag), 3.12.2001, Fakultät Chemie, Technische Universität München, Garching.

2.2.4 Scientific Committee

- R. Nießner: The Impact of (Bio-)Sensors and Bioanalytical Techniques on Environmental Monitoring. 5th Euroconference on Environmental Analytical Chemistry, 8.-12.09.2001, Blarney, Ireland: Scientific Committee.
- R. Nießner: New Trends and Needs for Chemical Field Screening. 2nd Int. Conf. Field Screening Europe 2001, 14.-16.05.2001, Karlsruhe: Scientific Committee (Chairman).
- R. Nießner: IUPAC International Congress on Analytical Sciences 2001, 6.-10.08.2001, Tokio: International Advisory Board Member.
- R. Nießner: Annual Meeting, Hydrochemical Society within the GDCh, 21.-23.5.2001, Bad Wildungen: Scientific Committee.
- R. Nießner, H. Puxbaum, M. Oehme: 2nd Workshop on Analytical Artefacts in Environmental Analysis and Related Areas (ARTEFACTA), 23./24.4.2001, Arlesheim, Switzerland: Scientific Committee.
- T. Baumann: AGU Spring Meeting, 29.5.-2.6.2001, Boston: Convener.
- U. Pöschl: European Aerosol Conference 2001, Leipzig, 3.9.-7.9.2001: Session Chair "Sulfur and Carbonaceous Particles"

2.2.5 Organisation of Scientific Meetings

- R. Nießner: 1st Late Summer Workshop, Interfaces in Aquatic Systems - Colloids, Biofilms, Sediment/Water/Air, 01.10-30.10.2001, Schloß Maurach, Germany.

2.3 Patents

- L. Kazarian, R. Nießner: Verfahren zum optischen Schalten und Drehschalter, Patent-Nr. 197 20 619, 1.3.2001, Deutsches Patentamt München.

2.4 Hydrogeological Consulting

Mineralisation control analyses Sibyllenbad, Endorf, Bad Birnbach, Bad Füssing, Bad Griesbach, Straubing, Gundremmingen,

Hydrogeological and hydrochemical expertises (mineral water, spa water) Bad Gögging, Bad Brückenau, Bad Wiessee, Bad Füssing, Kellberg, Erding, Bayreuth.

2.5 Diploma Theses

- Cand.geol. Marcus Bock: Tracerversuche zur Bestimmung des Wasser- und Stoffhaushaltes der MVA-Schlackedeponie Großmehring.
- Cand.chem. Michael Elsässer: Anwendung eines elektrischen Niederdruckimpaktors zur Aerosolcharakterisierung und Untersuchung von Cellulose-Partikeln.
- Cand.chem. Lillian Kleiber: Laserablation an heterogenen Feststoffproben.
- Cand.ing. Marcus Donié: Zeitaufgelöste laserinduzierte Fluoreszenzspektroskopie von Benzo[a]pyren auf Rußaerosolen (FH München).

2.6 PhD-Theses

Dipl.-Ing. Larissa Beier: Entwicklung, Bau und Anwendung der Lichtwellen-Multiplexer für faseroptisch geführte Sensorsysteme

Dipl.-Chem. Rüdiger Düsing: Multidimensionale Fluoreszenzspektroskopie in der Umweltanalytik

Dipl.-Chem. Andreas Exner: Einsatz der asymmetrischen Fluß-Feldflußfraktionierung in der Hydro-Kolloidanalytik unter Verwendung Thermischer-Linsen-Spektroskopie und anderer spektroskopischer Methoden zur Detektion

Dipl.-Chem. Lutz Krämer: Mikrostruktur ultrafeiner Aerosolpartikel und Photoakustische Detektion von Rußaerosolen

Dipl.-Min. Claudia Speiser: Exothermer Stoffumsatz in MVA-Schlackendeponien: Mineralogische und geochemische Charakterisierung von Müllverbrennungsschlacken, Stoff- und Wärmebilanz

Dipl.-Chem. Anne Zeck: Entwicklung von immunanalytischen, chromatographischen und massenspektrometrischen Methoden zur Bestimmung cyanobakterieller Hepatotoxine (Microcystine und Nodularine)

2.7 Habilitation Thesis

Dr. Michael G. Weller: Immunchemische Methoden in der Umweltanalytik

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
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
Massenspektrometrie in der Umweltanalytik	Weller, Nießner
Biochemische und molekularbiologische Analysenverfahren in der Umweltanalytik	Knopp
Die Mineral-, Thermal- und Heilwässer in Bayern und ihr hydrogeol. Rahmen	M. Baumann, Nießner
Einführung in das hydrogeologische Praktikum I, II, III	M. Baumann, Nießner
Brunnenbau und Bohrtechnik	M. Baumann, Nießner
Hydrogeologie I und II	Frisch (Lehrauftrag)
Ausbreitung von Schadstoffen im Untergrund	T. Baumann
Ausgewählte Kapitel und Übungen zur Hydrogeologie	T. Baumann
Erkundung und Sanierung von Grundwasserschadensfällen	T. Baumann
Modellierung der Grundwasserströmung und des Stofftransports	T. Baumann
Hydrochemische Modellierung	T. Baumann
Chemie und Technologie des Trink- und Betriebswassers I (Wasser und Umwelt)	Knopp
Chemische Charakterisierung von Umweltmatrices (Gase)	Nießner
Statistische Methoden in der Umweltanalytik	Panne
Umweltmeßtechnik mit spektroskopischen Methoden	Panne
Analytische Methoden für Gase und Aerosole	Pöschl
Gasmesstechnik	Pöschl
Atmosphärenchemie und Klimaforschung (TU Wien)	Pöschl

3.2 Lab Courses and Seminars

Vertiefungsfach Analytische Chemie, Teil 1 Organische Spurenanalytik	Nießner, Weller, Panne
Teil 2 Methoden der Strukturaufklärung und Instrumentellen Analytik	Nießner und Mitarbeiter, Dozenten in Garching
Wasserchemisches Praktikum I: Wasseranalyse	Panne, Weller, Nießner
Wasserchemisches Praktikum II: Wassertechnologie	Panne, Nießner
Praktikum Umweltmesstechnik	Pöschl
Bodenanalytisches Praktikum und Seminar (Univ. Konstanz)	Panne
Hydrogeologisches Praktikum I: Gesteinsphysikalische Methoden	M.+T.Baumann, Nießner
Hydrogeologisches Praktikum II: Hydrochemische Methoden	M. Baumann, Nießner
Hydrogeologisches Praktikum III: Geländeübungen mit Kurs	M.+T.Baumann, Nießner
Hydrogeologische und hydrochemische Exkursionen	M.+T.Baumann, Nießner
Hydrogeologisches, hydrochemisches und umweltanalytisches Seminar	M. Baumann, Nießner
Hydrogeologisches Literaturseminar	T. Baumann

3.3 Institute Colloquia

- H. Spitaler, Obmann der Kellereigenossenschaft Girlan/Bozen: Weinanbau zwischen Tradition und Fortschritt (26.1.2001)
- Dr. R. Noll, Fraunhofer Institut für Lasertechnik, Aachen: Neue Entwicklungen und Anwendungen der chemischen Direktanalyse mit Laser-Emissionsspektrometrie (7.2.2001)
- Dr. F. Stallmach, Institut für Experimentelle Physik I der Universität Leipzig: Einblicke in die Struktur poröser Gesteine mittels NMR-Techniken (19.2.2001)
- Prof. Dr. U. Stottmeister, Sektion Sanierungsforschung des UFZ Leipzig: Von der Sanierung einer Schwelwasserdeponie zum Implantat-gereigneten Biopolymer: Neue Wege der Biotechnologie für die Umwelt (26.3.2001)
- Prof. Dr. G.R. Fuhr, Institut für Biologie, Humboldt-Universität zu Berlin: Nutzung von Zellspuren für analytische Zwecke (28.3.2001)
- Dr. H. Grothe, Institut für Physikalische und Theoretische Chemie, TU Wien: Bildungsmechanismen für Polare Stratosphärische Wolken (20.4.2001)
- Prof. Dr. F. Arnold, Atmospheric Physics Division, MPI für Nulear-Physik, Heidelberg: Ionen in der Atmosphäre (8.5.2001)
- PD Dr. U. Karst, Lehrstuhl für Analytische Chemie, Universität Münster: HPLC/Elektrochemie/Massenspektrometrie-Kopplung und enzymverstärkte Lumineszenz von Lanthanoidkomplexen - Neue Ansätze in der Ultraspurenanalytik (14.5.2001)
- Prof. Dr. W. F. Rogge, Florida International University, Miami, USA: Residential Cooking: Emission Rates for TSP, PM10, PM2.5, Organic Compounds in PM 2.5, CO, NO and NO₂ (5.6.2001)
- Dr. R. Lohmann, Ralph M. Parsons Laboratory, MIT Cambridge, USA: The Real Partitioning of Dioxins and other Pollutants in the Environment (6.6.2001)

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- Prof. Dr. L. Yu, Dep. of Chemical and Environmental Engineering, National University of Singapore: Characterization of Nano-size Aerosols via AFM (20.6.2001)
- Dr. Y. Rudich, Dept. of Environmental Sciences, Weizmann Institute, Rehovot, Israel: Desert Dust Suppresses Precipitation - A Possible Desertification Feedback Mechanism (19.7.2001)
- Prof. Dr. S. Weinbruch, Institut für Mineralogie, TU Darmstadt: Elektronenmikroskopische Untersuchungen an atmosphärischen Aerosolpartikeln (14.8.2001)
- Prof. Dr. K. Therow, Universität Rostock: High-Throughput-Analytik für Synthese und Umweltapplikationen (30.8.2001)
- Prof. Dr. J. Pawliszyn, University of Waterloo, Canada: Solvent-free Sampling/ Sample Preparation Approaches Based on Fibre Geometry and Polymer Technologies (2.9.2001)
- Prof. Dr. D. Bursill, CRC for Water Quality and Treatment, Bolivar, South Australia: The Development of Cyanobacterial Research in Australia (19.10.2001)
- Prof. Dr. A. Seubert, Fachbereich Chemie, Philipps-Universität Marburg: Einsatz der On-line Kopplung Ionenchromatographie-Atom-spektrometrie für die Ultraspuren- und Elementspeziesanalyse (26.10.2001)
- Prof. Dr. J. Feldmann, Department of Chemistry, University of Aberdeen, Schottland: Speciation Analysis in Biogeochemistry: Challenge for the Analytical Chemist (26.11.2001)
- PD Dr. T. Kuhlbusch, FB9/Aerosolmesstechnik, Gerhard-Mercator-Universität Duisburg: Physikalische und chemische Charakterisierung von Partikeln in Emissionen und Immissionen (10.12.2001)

3.4 External Tasks and Memberships

Prof. Dr. Reinhard Nießner

IUPAC Commission V.4 Spectrochemical and Other Optical Methods of Analysis	Member
BayFORUV	Board of Directors
BayFORREST	Member
DFG SFB 411 Grundlagen der aeroben Abwasserreinigung	Member (until 6/2001)
Fachbereich IV Meßtechnik der VDI/DIN-Kommission Reinhaltung der Luft	Advisory Board Member
Bayer. Fachausschuß für Kurorte, Erholungsorte und Heilbrunnen	Member
Heinrich-Emanuel-Merck-Award	Jury Head
ISPAC-Award for Polycyclic Aromatic Hydrocarbon Research	Jury Member
Institute of Spectrochemistry and Applied Spectroscopy, Dortmund	Advisory Board Member
Institut für Abfallforschung, Augsburg	Advisory Board Member
Hydrochemical Society within the GDCh	Board of Directors
Association for Aerosol Research	Board of Directors
Analytical Chemistry	Associated Editor
Fresenius' Journal of Analytical Chemistry	Editorial Board Member
Mikrochimica Acta	Editorial Board Member
Römpp Lexika	Editorial Board Member
Fresenius' Environmental Bulletin	Advisory Board Member
Field Analytical Chemistry and Technology	Advisory Board Member
Analytical Sciences	Advisory Board Member
Analyst	Advisory Board Member

Dr. Manfred Baumann

Bayer. Fachausschuss für Kurorte, Erholungsorte und Heilbrunnen	Member
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PD Dr. Dietmar Knopp

BayFORREST	Member
DFG-SFB 411 Grundlagen der aeroben Abwasserreinigung	Member (until 6/2001)
KRdL-3/7/04, "Luftgetragene Mikroorganismen und Viren", im VDI/DIN	Member
Vom Wasser	Editorial Board Member

Dr. Ulrich Pöschl

Atmospheric Chemistry and Physics	Chief Executive Editor
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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.

Three field sites equipped with more than 100 monitoring wells and carefully hydrogeologically and hydrochemically characterized are available for field scale propagation studies.

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

- 4 He/Ne-laser
- 6 Nd-YAG-laser
- 1 CO₂-laser
- 3 Dye-laser (tuneable with frequency doubler)
- 5 N₂-laser
- 8 Tuneable diodelaser (600-1670 nm; ca. 100 mW CW)
- 1 Laserdiodearray 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
- 1 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 oszilloscopes (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 chromatographic system
- 3 HPLC, UV/VIS array detector, programmable fluorescence detector
- 2 HPLC
- 1 Capillary electrophoresis system
- 1 Ion chromatograph, Dionex 4500 i



- 1 Ion chromatograph, Dionex 14
- 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 Flammen-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

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

4.2.8 Sum Parameters

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

4.2.9 Aerosol Research



- 1 Aerosol chamber (1 m³)
- 1 Aerosol flow tube (10 L)
- 1 Ozone analyzer (UV absorption)
- 1 NO/NO₂ analyser (Chemiluminescence)
- 2 Aerodynamic particle sizers (0.5-25 μm)
- 1 Berner impactor (9 stages, 50 nm - 16 μm)
- 1 Electrical low-pressure impactor (12 stages, 30 nm - 10 μm)
- 2 Low-Volume filter samplers (PM 10, PM_{2.5})
- 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 Brush aerosol generator (powder dispersion)

4.2.10 Pilot scale lab

View from the top:



5 Staff 2001

Univ.-Prof. Dr. Reinhard Nießner

Dr. Manfred Baumann
Dr. Thomas Baumann
Dr. Christoph Haisch
Dr. Monika Hamers-Schneider (until 11/01)
Dr. Stefan Kamm
Dr. Dietmar Knopp
Dr. Kerstin Krause (from 8/01)
Dr. Nikolaus Nestle
Dr. Ulrich Panne
Dr. Ulrich Pöschl
Dr. Michael Weller

Birgit Apel
Günter Dollinger
Roswitha Glunz
Irmengard Kefer (until 12/01)
Karin Koller
Gisela Lang
Joachim Langer
Ramona Leube (from 8/01)
Susanne Mahler
Christine Sternkopf
Christa Stopp
Sebastian Wiesemann

Hatice Hazir
Mira Kolar

PhD Students

Dipl.-Geol. Matthias Alte (from 8/01)
Dipl.-Chem. Harald Beck
Dipl.-Chem. Petra Degelmann (from 8/01)
Dipl.-Chem. Marcus Diemer (until 9/01)
Dipl.-Chem. Barbara Fall
Dipl.-Chem. Herbert Fink
Dipl.-Chem. Thomas Franze
LA Sabine Hegendorf (until 9/01)
Dipl.-Geol. Ralf Klein
Dipl.-Chem. Bertram Knecht (from 4/01)
Dipl.-Chem. Lutz Krämer (until 3/01)
Dipl.-Chem. Marion Lackhoff
Dipl.-Chem. Thomas Letzel (until 1/01)

Dipl.-Ing. Armin Messerer (from 10/01)
Dipl.-Chem. Harald Prestel (until 5/01)
Dipl.-Phys. Igor Radivojevic
Dipl.-Geol. Angelika Reisinger (2/01-6/01)
Dipl.-Geol. Maik Sarnes (until 5/01)
Dipl.-Chem. Tim Scharnweber (until 2/01)
Dipl.-Chem. Christian Schauer
Dipl.-Leb. Isabel Schaupt
Dipl.-Chem. Matthias Schedl (until 8/01)
Dipl.-Chem. Thomas Schmid
Dipl.-Chem. Martin Schweigkofler
Dipl.-Chem. Mario Seiss (until 7/01)
Dipl.-Geol. Dagmar Spangenberg (from 9/01)
Dipl.-Chem. Carola Wersching
Dipl.-Chem. Anne Zeck (until 9/01)
Dipl.-Chem. Axel Zerrath

External PhD Students

Dipl.-Biol. Thomas Meindl (GSF)
Dipl.-Chem. Norbert Uwe Kemnitzer (until 7/01)
Dipl.-Chem. Dieter Rothe (MAN)
Apothekerin Ellen Bitterle (GSF)

Diploma Students

Cand.chem. Michael Elsässer (3/01-9/01)
Cand.chem. Lillian Kleiber (6/01-11/01)
Cand.ing. Marcus Donié (until 4/01)

Guests and Research Fellows

Xavier Prieto-Mollar (Uni Barcelona/Spainien)
Dr. Constantine Stalikas (University of Ioannina/Greece)
Dr. Qing-Zhi Zhu (Xiamen University/China)

Student Assistants

Christian Gerlach (from 8/01)
Johanna Kirstein (4/01-6/01)
Simon Pfanzelt (5-7/01)
Christine Eilender (7/01-8/01)
Clemens Helmbrecht (from 9/01)
Andreas Keilbach (from 12/01)