

# Annual Report 2016

Institute of Hydrochemistry Chair of Analytical Chemistry



Members of the IWC in December 2016

Institute of Hydrochemistry Chair of Analytical Chemistry Technische Universität München Marchioninistr. 17 D–81377 München http://www.ws.chemie.tu-muenchen.de

Editor: Dr. Thomas Baumann



# **Editorial**

Dear colleagues and friends!

This editorial is my last one, written at the end of my active period of employment. In November 1989 I became appointed Full Professor for Hydrogeology, Hydrochemistry and Environmental Analytical Chemistry at my present location Technical University of Munich (TUM). Today I am looking back on a long period of time, full of expectations, visions, some disappointments, and many success stories.

At the end of 80ies I became aware of the beautiful analytical possibilities of antibodies, and was fascinated from the very beginning. Up to now I'm still very convinced of this technology. I had the luck to find extremely talented and competent coworkers as group leaders in this field of bioanalysis, like Profs. Dietmar Knopp and Michael Weller, who made this part at IWC extremely successful and widely recognized. Apart from flying to Mars, some of our monoclonal antibodies are still in use worldwide by many institutions. Today, this field of research is driven by PD Michael Seidel, who is currently optimizing and extending bioanalysis at IWC towards microarray technology, standing out with the release of the known platform MCR3 (Munich Chip Reader, series 3), an autonomously operating microarray analysis device

The other branch of IWC is the applied laser spectroscopy. We started (under the leadership of Prof. Ulrich Panne and PD Christoph Haisch) with laser breakdown spectroscopical process analysis and fiber-optically guided, time-resolved laser fluorescence sensing. Depth-resolved photoacoustic spectroscopy allowed the direct time-resolved observation of biofilms, and even monitoring the glucose level in human tissue. Many well cited papers document this period. A certain highlight was the establishment of the gold standard for soot measurement in combustion engine exhaust, a photoacoustic spectrophone for online measurement, nowadays known all over the world as *Micro Soot Sensor*<sup>™</sup>.

Particles in all varieties were and will be strong field of expertise of IWC. Not only hydrocolloid size characterization by flow field technologies and laser light, but also by Raman microspectroscopy brought us to the forefront in this area (pathogenic bacteria & biofilms). The basics for the characterization of soot particles from diesel engine with Raman spectroscopy were developed here. This ground-breaking paper, written by the former group head Prof. Ulrich Pöschl, will reach 1000 citations this year. Just now another technique, the unambigious characterization of microplastic by Raman microspectroscopy developed in the group of Natalia P. Ivleva, makes its way into the laboratories and standards.

Starting this century, we were among the first, to visualize and quantify colloid and contaminant transport processes *in situ* and online using Magnetic Resonance Imaging in PD Thomas Baumann's group. Antibodies coupled to super-paramagnetic nanoparticles allowed a selective visualization of contaminants, even if those did not alter the magnetic field.

Currently the transition to my successor, Prof. Martin Elsner, renowned for stable isotope mass spectrometry, who will follow me April 1, 2017, as Full Professor and Head of the IWC, takes place. He is inherting a strong team to accompany his research and to explore new fields around nanoparticles, bacteria, and bioreceptors.



To this end, I spent a fruitful and very satisfying period of my life at IWC, with so many supportive colleagues and enthusiastic students. So far, about 150 PhD students, and approx. 200 Master students finished their thesis at IWC within my working period. Many thanks to all of them! I hope, I could contribute a little bit to their success with not too many crazy ideas and visions. Eventually, it seems, most of them became reality sooner or later.

Thanks also to all the hidden members of the club, the technicians and secretaries, who had to catalyse daily life! And, last but not least, my cordial thanks to my faculty at TUM, and our "Kreis der Freunde des Instituts für Wasserchemie und Chemische Balneologie" ("Circle of friends of the IWC").

Thank you very much and take care!

**Reinhard Niessner** 

# Hydrogeology and Hydrochemistry (PD Dr. T. Baumann)

## **Changes of Nanoparticles Along Their Life-Cycle**

Funding: DFG (Deutsche Forschungsgemeinschaft) Cooperation: DFG Research Unit InterNANO (FOR1536)

The application of nanoparticles in various sectors and consumer products continues to increase in a rapid pace. Silver and titanium dioxide nanoparticles are among the engineered nanomaterials that are very often incorporated in a wide variety of consumer products. The widespread use of silver and titanium dioxide nanoparticles is mainly due to their higher antimicrobial activity relative to their bulk materials. However the large scale applications of these two nanoparticle types increase the likelihood of human exposure and also the potential for their release to the environment which leads to subsequent impacts on biotic and abiotic processes in those environments.

The environmental fate and biological effects of nanoparticles is dependent on several different factors such as interactions with dissolved organic matter (DOM), multivalent cations and natural colloids as well as homo-aggregation, hetero-aggregation and also chemical transformation. A general understanding of these mechanisms and also interactions between nanoparticles and their coating is required in order to predict the fate, stability and toxicity of nanoparticles.

Surface-enhanced Raman scattering has been shown as a sensitive and selective method for the characterization of natural coatings on noble metal nanoparticles like silver or gold. The enhancement factors on noble metal nanoparticles can reach  $10^8$  to  $10^{11}$ . Although enhancement factors of  $10^2$  to  $10^4$  have been reported and measured for semiconductor based nanoparticles, a direct characterization of coatings on semiconductor nanoparticles like  $\text{TiO}_2$  is not straightforward. The signal enhancement on semiconductor nanoparticles is dependent on several factors such as size, surface defects, shape, and surface morphology of the nanoparticles. The coating of the nanoparticle also plays an important role on the possibility of the enhancement.



Workflow for the detection of 4-MBA on thermally modified TiO<sub>2</sub> nanoparticles

In order to characterize the formation and stability of coatings on TiO<sub>2</sub> nanoparticles, we thermally modified P25-TiO<sub>2</sub> nanoparticles at different temperatures and coated them with 4-Mercaptobenzoic acid (4-MBA) as a sample organic matter. Results show that the enhancement factors increase on thermally modified nanoparticles and 4-MBA coatings can be detected. The 4-MBA coating is shown to be stable for at least six steps of washing steps (centrifugation and resuspension in deionized water). *S. Amininejad, N. P. Ivleva* 

## Mass Transfer at Interfaces to Non-Aqueous Phases

Funding: TUM International Graduate School of Science and Engineering (IGSSE) Cooperation: Prof. Manhart, Chair of Hydromechanics, TUM

Mass transfer in porous media is relevant in many environmental applications and provides the basis for numerous technically relevant processes of material seperation and conversion. The mass transfer at fluid interfaces is associated with interface convection caused by local inhomogeneities in interface tension and hydrodynamic

in interface tension instabilities at the interface. If there is a surface tension gradient along the surface a shear stress jump is generated that results in fluid motion along the surface that is called Marangoni effect. These spontaneous convection currents can lead to an increased mass transfer of the transition component at the phase boundary and to an increased mixing of water with high temporal and spatial resolution. The use of fluorescent particles as well as the recording and analysis of their trajectories is intended to visualize interfacial processes and to quantify the mass transfer at fluid phase boundaries. Concentration gradients at the interface are analyzed by spectroscopic methods and allow an

assessment of the

phase boundaries.

series provide the

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for quantifying and

analyzing the impact of the Maran-

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Microscopic image of an 1-octanol-water-air interface in a microfluidiic channel

the phases. Therefore compensatory currents along the interface can have a significant influence on the efficiency of several process applications and on the subsurface transport of contaminants in the groundwater.

Using microfluidic channels and advanced experimental techniques it is possible to measure the fluid flow and mass transfer rates at these interfaces directly and to quantify the effect of the Marangoni convection on the mass transfer rates at interfaces between a nonaqueous liquid and we concentrate on the effect of Marangoni convection on the mass transfer near an 1-octanol-water interface, which serves as a well defined proxy for nonaqueous phase liquids (NAPL) in porous media. Experiments and a numerical simulation are closely coupled to provide a generic data set with high reproducibility and used to obtain highly resolved three-dimensional data of mass transport in two- and three-phase systems. *C. Wismeth* 

## **Scalings in the Geothermal Cycle**

Funding: BayMWi (Bavarian State Ministry for Economy), Geothermie-Allianz Bayern Cooperation: Operators of geothermal facilities in the Bavarian Molasse Basin

Scalings are a widespread problem for the geothermal plants which exploit the Malm Aquifer in the Bavarian Molasse Basin. They affect the technical and economic efficiency and cause costly revisions of the facilities throughout the complete geothermal cycle. Scalings observed mainly consist of different CaCO<sub>3</sub> polymorphs and are found in the production well, at the motor, in the pumps

and pipes and throughout the groundlevel facilities including the heat exchangers.

The two main processes responsible for the formation of scalings are local temperature peaks and degassing of less soluble gases due to local pressure drops. While the increase of

the temperature leads to a local supersaturation at the hot surfaces of e.g. the motor, the formation of gas bubbles strips soluble gases (i.e.,  $CO_2$ ) from the solution. Here, the carbonate-equilibrium is shifted to higher pH-values and less soluble carbonates.

So far, scalings were collected from the pumps and the production pipes after necessary exchanges of the submersible pumps, from the particle filters, in the groundlevel geothermal facilities, and from the injection pipes. The samples were characterized by SEM-EDX, XRD, and image processing to assess the mineralogical features and the elemental composition. The



Scalings in an injection pipe (photo: Seitz-Gutmann)

porosity and bulk density were measured to assess the mass of the deposits and to calculate the kinetics of the formation. All together, this generated a unique quantitative dataset with a spatial resolution of 9 m along the production tubes.

In the production pipes, the scalings at the well head show a crystalline structure with little porosity, the scalings at the pump

> reveal a structure found usually in pumice. The overall thickness correlated to the produced volume of thermal water and is on the order of 500-1500 µm/10<sup>6</sup> m<sup>3</sup>. There was a significant difference of the scaling thickness above the pump at comparable production volumes. This

might be attributed to either the type of pump or to the number of starting cycles.

Scalings in the ground-level facilities at one site were composed of small grains cemented with thin layers of carbonates. Here, the structure and composition of the scaling and the hydrogeochemical model suggest, that the cementation took place during maintenance. The scalings were likely mobilized during start-up after maintenance and accumulated at the inlet to the heat exchanger blocking the exchanger pipes. To prevent this type of scalings the maintenance procedure has to be revised.

B. Köhl

## **High-Temperature-Aquifer Storage**

#### Funding: BMW (BayINVENT)

Cooperation: TUM Hydrogeology; Erdwerk GmbH, Munich; Aquasoil GmbH, Berlin

Combined heat and power plants (CHP) are efficient and environmentally friendly because excess heat produced during power generation is used for heating purposes. While the power demand remains rather constant through-out the year, the heat demand shows seasonal variations. In a worst-case scenario, the heat production in

winter is not sufficient, and the power production in summer has to be ramped down because the excess heat cannot be released the environment. to Therefore, storage of excess heat of CHP is highly beneficial from an economic and an ecological point of view.

Aquifer thermal energy storage is considered as a promising technology for energy storage. In a typical setting, water from an aquifer is

produced, heated up by excess heat from the CHP and injected through a second borehole back into the aquifer.

The carbonate rocks of the upper Jurassic seem to be promising sites for aquifer heat storage because of their high transmissivity combined with tight caprock in a typical geological setting. However, reactions in the aquifer cannot be neglected and may become the limiting process of the whole operation. While there have been several studies performed in clastic aquifers and for temperatures below 100 °C, the knowledge

about high injection temperatures and storage into a carbonatic aquifer matrix is still limited.

Within a research project funded by the Bavarian State Ministry for Economic Affairs and the BMW Group, the storage and recuperation of excess heat energy into the Upper Jurassic aquifer at flow rates of 15 L/s

> and temperatures of up to 110 °C was investigated. The addition of CO<sub>2</sub> was used to prevent precipitations. Data from the field site was backed up by autoclave experiments and used to verify a conceptional hydrogeochemical model for the heat

model for the heat storage operation. The model allows to parametrize the operation and to predict possible reactions in the aquifer.

In the course of the heat storage test the crystallisation processes of the polymorphic forms of calcium carbonate were investigated. Complementary laboratory experiments in an autoclave were run. The results indicate that turbulent flow regime during the heat storage test inhibited the crystallisation of aragonite up to temperatures of 100 °C and calcite crystallisation was favoured by strong diffusion gradients even at high temperatures.

M. Ueckert



Calcite particles formed during the heat storage test

## Large Scale Geothermal Exploration in the Molasse Basin

### Funding: Exorka (BayINVENT)

Cooperation: LIAG Hannover; Exorka, Grünwald

The carbonaceous sediments of the Upper Jurassic aquifer in the Bavarian Molasse Basin are one of the most promising regions for geothermal energy usage in Germany. Especially the greater Munich area is a promising region for geothermal exploration. The Upper Jurassic sediments are dipping towards the alps, hence significantly higher temperatures can be produced in the southern part of Munich compared to the northern part.

Therefore, the northern part of Munich with temperatures of 70 - 90 °C is mainly used for locally confined district heating. After the heat extraction, the water has a temperature of about 50 °C and is reinjected into the aquifer. In the southern part, water with temperatures 125 - 140 °C serves for power generation. Here, the water is reinjected with temperatures of about 80 °C into the aquifer. To this end, these temperature levels could still be used as a geothermal ressource in the northern part.

The project "GeoWärme München" looks at a more efficient exploitation of geothermal energy by coupling a geothermal doublet system in the southern part with a geothermal doublet system in the northern part. The aim is to use both bore holes in the south to produce hot water, run a geothermal power plant and to pipe the water after the first heat extraction via a district heating system into the north of Munich. Along the pipeline several other heat exchangers are coupling out heat for district heating and process heat. Since now the double amount of heat is available, there will still be sufficient heat for the facility in the north where the cold water is injected. In total one could expect an increase in efficiency of about 70%.

The increased production rates at one geothermal site as well as the increased injection rates 30 km downstream could result in large-scale hydraulic changes which have to be assessed carefully. Changes of



Schematic of the regional exploration of geothermal energy by coupling higher enthalpy wells in the South with lower enthalphy drillings in the North

the stress implied on the formation have to be considered to assess the long-term hydraulic and geotechnical properties of the reservoir rocks. Also, based on our analyses, the hydrochemical conditions are different for the different wells, which might cause some problems for the ground level facilities. The results from the Pullach site, however, indicate a benign behaviour of the mixed and cooled water, once injected into the reservoir.

M. Ueckert

### Bioanalytics (Apl. Prof. Dr. D. Knopp)

# Development and validation of an immunological screening method for the determination of toxicologically relevant pyrrolizidine alkaloids in herbal tea and related matrices

Funding: FEI – Research Association of the German Food Industry (AiF 19010N) Cooperation: Lehrstuhl für Lebensmitteltoxikologie der LMU München, Prof. Gareis, Dr. C. Gottschalk, F. Kaltner

Pyrrolizidine alkaloids (PAs) are so called secondary metabolites and therefore classified as naturally occurring alkaloids. More than 660 PAs including corresponding Noxides (PANOs) are identified in more than 6000 plants leading to a worldwide distribution.

Their chemical structure is based on a pyrrolizidine ring and each PA can be derived



Chemical structures of relevant pyrrolizidine alkaloids. Pyrrolizidine ring (a); basic structures/necine bases (b); monoester, diester and PANOs (c)

from one out of three basic structures (necine bases) named Retronecine, Heliotridine and Otonecine. Esterification of the primary or secondary hydroxyl group, leading to mono-, diesterified, or even cyclic structures, results in a huge structural variety. In the liver, PAs can be metabolized by cytochrome P450 to highly reactive pyrrole esters, which are able to build harmful DNA and protein adducts.

The food industry is highly interested in an in-house method for fast, easy, and effective analysis of unprocessed plant resources and other raw materials in order to assess the PA content.

Bioanalytical methods based on immunological detection of the analyte are most suitable in this context, as they provide parallel processing of many samples and require minor trained staffing. Moreover, they are cheap and do not require any costly sample preparation. In order to address food industries demands, the aim of this project is to develop and validate an immunological screening method for the determination of toxicologically relevant PAs in herbal tea and related matrices.

While previous investigations were focused on the generation of polyclonal antibodies against PAs, the current project aims at the generation of monoclonal antibodies. Relevant basic structures are used as haptenes for derivatization using appropriate coupling chemistry. After characterization of synthesized derivates using ESI-MS, and covalent coupling to protein carriers, the substitution grade was determined using MALDI-TOF-MS. Mice were immunized and sera were tested regarding antibody titer and selectivity. Suitable mice were used for hybridoma technique and cell culture supernatants were extensively screened for suitable cell clones. Chosen cell clones were used for the generation of monoclonal antibodies.

# Plant-Produced Antibodies for the Depletion of MC-LR, the Most Toxic Cyanotoxin Congener Produced by Blue Algae

#### Funding: DFG (Deutsche Forschungsgemeinschaft)

Cooperation: University of Natural Resources and Life Sciences (BOKU), Vienna, Austria, Prof. Dr. E. Stoeger

Eutrophication of surface waters caused by the enrichment of some nutrients and also higher temperatures can promote cyanobacterial (blue-green algae) blooms, which is a worldwide environmental problem. Many of the cyanobacterial species are able to produce potent cyanotoxins.

Microcystin-leucin-arginine (MC-LR) is the most frequent and most toxic microcystin congener. Commonly used methods for the removal of extracellular MC-LR in water can be separated into chemical oxidation and physical methods, which are partially accompanied with disadvantages, above all a low selectivity.

Another option is the use of biological receptors, e.g., using genetically engineered plants with extended remediation capabilities under environmental conditions or trapping the target analyte using biofilters based on immunoextraction technology. This project, for the first time, focused on the preparation of purified plant-derived antibodies for the concentration of MC-LR from aqueous environmental samples.

Following the generation of the plantibody in tobacco plants, its detailed characterization and comparison with its murine original antibody using ELISA and Surface Plasmon Resonance Spectroscopy (SPR) was performed in fundamental studies to estimate specificity, kinetic constants and matrix interferences. For example, experiments showed the high stability against chaotropic ions, organic solvents, humic acids and stability of the plantibody over a wide pH-range. The focus of the final project period was put on investigations regarding principal applications of the plant-derived antibody as a bioremediation reagent in terms of sol-gelbased biofilter material.



Schematic of the plantibody setup

Depletion experiments were conducted with spiked surface water samples under different modes like sequential sample addition, continuous cycling mode and suspension method and resulting binding capacity and necessary depletion time compared. In addition, plantibodies obtained with different purity were tested for practical application. *A.-C. Neumann* 

# Applied Laser Spectroscopy (PD Dr. C. Haisch)

### Photoacoustic Spectroscopy in Mixed-phase Dispersions

#### Funding: Alexander von Humboldt-Foundation

Cooperation: TU Berlin, Institut für Optik und Atomare Physik, LMU LIFE-Centre Laser-Forschungslabor

Gold nanoparticles can be used as exogenous contrast agents for biomedical photoacoustic imaging, which is an emerging hybrid biomedical imaging modality combining optical and ultrasound imaging, yielding advantages of spectroscopic contrast with high-resolution deep-tissue imaging capability.



Schematic for photoacoustic sensing of a multi-phase dispersion

In photoacoustic imaging, absorbed light energy is converted to acoustic wave energy, which can be measured using ultrasound detectors. Advantages of using gold nanoparticles as contrast agents include high absorption due to surface plasmon resonance, tunable spectra based on particle size and shape, excellent biocompatibility, and the possibility to add various surface functionalities.

This project examines the photoacoustic signal generation efficiency in suspensions of gold nanospheres in water, with the goal of future quantitative biomedical enabling photoacoustic imaging of nanoparticles. Systematic series of photoacoustic experiments were performed using suspensions of gold nanoparticles in a backward-mode photoacoustic sensor with laser excitation at 532 nm from a nanosecond pulsed Nd:YAG laser. The dependence of the photoacoustic signal on variables such as the particle diameter, optical density, excitation fluence, and silica coating thickness were quantitatively investigated. To correlate the generated photoacoustic signal generated with the absorbed optical energy, an integrating sphere setup designed for measuring optical properties of scattering media was employed to differentiate optical absorption and scattering.

The results of this study add new evidence to the understanding of the processes involved in the generation of photo-acoustic signals from gold nanospheres. The findings can be applied to advance the application of nanospheres as contrast agents in photoacoustic imaging in bio-medicine, and may facilitate their future application in molecular and quantitative photoacoustic imaging studies. *G. Pang* 

# Laser Photofragmentation for the Detection of Nitro-PAHs in Combustion Engine Exhaust

Funding: DFG (Deutsche Forschungsgemeinschaft)

Nitrated polycyclic aromatic hydrocarbons (NPAHs), together with their parent compounds, PAHs, are probably the abiotic class of substances which is most harmful for human health, not only in the atmosphere, but in the total environment. More than a third of the mutagenic potential of ambient air is attributable to NPAHs.

Our aim is to employ photofragmentation (PF), the process of breaking chemical bonds through interaction with one or multiple photons, as a means to investigate NPAHs in the gas phase as well as adsorbed on aerosol particulate matter. High sensitivities in the low ppb- or even ppt-range for PF-based gas phase analysis can be achieved.

Different modalities can be distinguished, regarding the fragmentation mechanism and the way of fragment detection. Resonant fragmentation allows for a rather straightforward system setup; a single laser pulse can be employed for fragmentation and photoionization. Depending on the photon energy employed, the fragments can be generated in an excited state, relaxing by optical emission.

For nitrated aromatic compounds, a fragmentation process including elimination of nitrogen dioxide  $(NO_2)$  in an excited state and consecutive decay to excited atomic oxygen and excited nitric oxide (NO) is known. The excited NO molecules optically

relax to the ground state.

A frequency-doubled optical parametric oscillator pumped by the third harmonic of a





pulsed Nd:YAG laser is used as a light source with a broad continuous tuning range in the ultraviolet as well as visible spectral range. Spectral resolution and detection is carried out by a grating monochromator and a photomultiplier tube. Additionally, mass spectrometry is employed as reference analysis.

S. Schneider

## Antibiotic Resistance Testing of Urinary Tract Infection Bacteria by Surface Enhanced Raman Spectroscopy

Funding: DFG (Deutsche Forschungsgemeinschaft), China Scholarship Council (CSC, grant for Li Qiu)

Cooperation: Prof. Stief, Urologische Klinik der LMU München; PD Dr. Wieser, Max von Pettenkofer-Institut, LMU

Fast analysis and test methods for microorganisms are urgently needed in order to allow for a timely and efficient treatment. Urinary tract infection (UTI) is one of the most frequently occurring bacterial infections worldwide and thus represents a heavy burden on the healthcare system. As it is



Potential workflow for the fast antibiotic resistance testing of bacteria by SERS.

generally known, the number of antibiotic resistant bacteria is constantly increasing and hence, antibiotic resistance testing is vital. However, up to date testing procedures are time consuming, mostly since they require for cultivation prior to testing.

Recently, we presented a SERS- (surface enhanced Raman scattering) based procedure to distinguish living and dead bacteria, using an *in situ* silver colloid formation on bacteria. This approach promises to be suitable for a very fast testing within few minutes and it can be applied on single organisms, if necessary, making cultivation obsolete.

However, it is a large step from our first proof of concept to a routine application under real-live conditions. The aim of the project is to fully investigation the feasibility of this test with real samples, a range of clinically relevant antibiotics and bacteria species and strains. In particular, we need to find a means to make this approach also applicable for gram-positive organisms, where our preliminary tests were not all to successful. The influence of the biological matrix containing the bacteria has to be investigated and suitable sample preparation methods will be developed in order to allow for successful use independent on the chemical environment of the sample. Also, we are working on a sampling platform for the handling of the sample, which is suitable for the sample pre-treatment as well as for the Raman-microscopic investigation. The test conditions will be elaborated in close collaboration with the project partners, which guarantees a sustainable work procedure. Finally, the capacity of the method shall be tested in comparison with routine analysis and thus the applicability of the method can be evaluated.

L. Qiu, D. Bauer

# Sampling and Detection of N<sub>2</sub>O in Wastewater Treatment Plants

Funding: International Graduate School of Science and Engineering (IGSSE) Cooperation: TUM, Chair of Urban Water Systems Engineering, Prof. Drewes

Nitrous oxide (N<sub>2</sub>O) is a strong greenhouse gas with a significantly higher global warming potential than carbon dioxide. N<sub>2</sub>O is produced by wastewater treatment plants (WWTPs) during the biological nitrogen removal process. Due to the lack of comprehensive monitoring approaches there is limited data available to establish quantitative relationships between nitrous oxide emissions and process parameters of biological nitrogen conversions. The goals of this project are to develop novel monitoring and control strategies for N<sub>2</sub>O employing photoacoustic (PA) laser spectroscopy. That will enable a tight control of contemporary nitrogen removal processes as well as new ways in harvesting N<sub>2</sub>O for enhanced energy recovery from waste streams.

Together with the chair of Urban Water Systems Engineering, an appropriate gas capture and conveyance system has been developed. Gas samples from multiple testreactors are continuously pumped to the central PA-based detection unit, where N<sub>2</sub>O is measured sequentially. In addition, a novel sample device comprised of a highly selective gas permeable membrane, which is submerged in the mixed liquor reactor, has been developed to extract N<sub>2</sub>O from the liquid phase. The subsequent gas-phase analysis is performed by photoacoustic spectroscopy. Dimensions of the gas permeable membrane, as well as the gas flow have been optimized. We compared different theoretical calculations of the extraction efficiency, based either on a straightforward mathematical model or on a finite element simulation. Based on the outcome, a field

probe was developed and tested on a WWTP, yielding results comparable to the one achieved by gas-chromatographic reference analysis.

Other approaches for dissolved  $N_2O$  detection involve degasification methods. We tested degasification by pressure reduction, degasification by aerosol generation and gas-



In-house developed gas sampling hood in action at a wastewater treatment plant

stripping. Extraction efficiency was compared and the combination with the PA-setup for online  $N_2O$  detection was tested.

Tests of the PA setup under real conditions at a wastewater treatment plants were performed. A sampling hood was placed in the reactor of a full-scale wastewater treatment plant. In combination with an electrochemical  $N_2O$  sensor simultaneous determination of  $N_2O$  in the liquid and in the gas phase was possible. A complete characterization of  $N_2O$  emission during nitrogen removal process was determined. *K. M. Thaler* 

# Down to Ten - Characterization of Combustion Engine Exhaust Particles in the Size Range from 10 to 23 nm

#### Funding: European Union

Cooperation: Aristotle University of Thessaloniki, AVL List GmbH, Ricardo UK Ltd, Tampere University of Technology, Graz University of Technology, Joint Research Center, Centro Ricerche FIAT SCpA

DownToTen seeks to develop a reliable and robust methodology to enhance the regulatory approach in the assessment of particle number emissions in the sub 23nm region (down to at least 10nm), focusing on state-ofthe-art automotive powertrains with direct in-



Soot particles, electrostatically deposited for off-line analysis

jection gasoline engines, but also diesel engines, under real-world operation conditions. To this end, DownToTen will first investigate and quantitatively describe the nature and the characteristics of nanoparticles <23 nm (formation, origin, physical and chemical characteristics), and will set up a synthetic aerosol bench for fundamental studies at instrument level for the facilitation of metrology and evaluation purposes. Existing, proposed and under development instruments will be evaluated against rigorous criteria for the measurement of sub-23 nm particles, with emphasis on their applicability as portable emissions systems (PEMS).

Our task within this project is the chemical characterization of the sub-23 nm particles by various techniques. Potential candidates for an off-line analysis scanning electron microscopy SEM in combination with EDX dispersive x-ray fluorescence), (energy temperature programmed oxidation (TPO), and NAA (neutron activation analysis). However, artefact-free sampling of nanoparticles is a challenge, hence we also employ online analytical techniques, which are developed within the framework of the project. Photoacoustic soot sensing will be combined with a specially developed soot reactivity sensing device. Mass spectrometry with a new ionization source from Plasmion, a high-tech start-up company founded by alumni J.-C. Wolf, allows for direct online analysis of exhaust gas. It will be combined with particle size fractionation and an evaporation, thus allowing for the characterization of volatile and semi-volatile particles. K. M. Thaler, A. Rinkenburger

# Raman Microspectroscopy (Dr. N. P. Ivleva)

### Fibers in Beverages: Raman Microspectroscopic Analysis

Funding: IWC

Microplastic (1 µm – 5 mm, MP) has become an emerging topic in recent years. Severe effects on the health of different aquatic organisms after the ingestion of MP have been shown. For humans these effects cannot yet be proven nor declined. In this context a report on MP fibers in German beers attracted high interest. In this study fibers were identified by optical microscopy leaving doubts about the origin and transfer pathways of the detected fibers. Optical identification cannot unambiguously differentiate between synthetic polymer fibers and harmless cellulose fibers. The composition of fibers, hence, has to be examined with advanced spectroscopic techniques.

Raman microspectroscopy (RM) is an established method for MP analysis. It combines Raman spectroscopy, which is based on the inelastic scattering of light, and an optical microscope. It features several advantages like the non-invasive and non-contact analysis of particles with a spatial resolution down to 1  $\mu$ m. The identification is conducted via the resulting fingerprint spectra which are unique for the different polymer types.

In our study, we performed a qualitative and quantitative analysis of fibers collected from beer and bottled mineral water by means of RM. We focused on illustrating contaminations and possible prevention methods. The sample preparation was performed in a laminar flow box and blanks were taken for every beverage sample and the air in the laminar flow box. We found cellulose and MP-fibers in an arbitrary manner throughout the beverage samples and the respective blanks. Besides the use of a laminar flow box these contaminations could not be prevented. As possible sources



Unambiguous identification of a cellulose fiber stained with indigo by Raman microspectroscopy

for the contamination, the filter packaging, which contains polyethylene, the most often found polymer in our study and laboratory air were identified. We therefore could show that mere optical identification alone is insufficient and blank filters are indispensable for the analysis of MP. To this end, our results cannot confirm a contamination of beverages with synthetic fibers.

P. M. Anger, A. C. Wiesheu, T. Baumann

# Microplastic in the Water Cycle – Sampling, Sample Preparation, Analysis, Occurence, Removal and Evaluation (MiWa)

### Funding: BMBF (Federal Ministry for Education and Research) Cooperation: Technical University of Berlin, Prof. Jekel, Dr. Ruhl; BAM (Bundesanstalt für Materialforschung und –prüfung), Dr. Braun; Hochschule Fresenius, Dr. Klein; Umweltbundesamt, Dr. Bannick; Water Technology Center Karlsruhe, Dr. Storck; Berliner Wasserbetriebe, Gnirß; Helmholtz-Centre for Environmental Research, Prof. Reemtsma, Dr. Wagner; Umweltbundesamt, Dr. Grummt; Eberhard Karls Universität Tübingen, Prof. Triebskorn; Goethe University Frankfurt, Dr. Wagner; Heidelberg University, Prof. Braunbeck

Microplastic (MP), a term used for particles methods and biological data for various made of synthetic polymers with a size below species.

5 mm, became a topic of public concern in the last years. Synthetic polymers are important materials in our daily life. They exhibit many advantages over alternative materials, e.g. their low weight.

However, the release of litter containing MP poses a threat to the environment. Although its impact on nature is still a field of debate, concerns rose. It was shown that MP can be uptaken by different species from Daphnia magna to bivalves and fish and can have severe effects on their health. These effects may arise from

physical damage in the digestion tract or due to hazardous substances or (potentially) pathogenic bacteria adsorbed on the MP particles.

The project MiWa (Microplastic in the Water Cycle) aims to give a first comprehensive evaluation of MP in the water cycle. This evaluation will include data of the MP occurrence determined by different analytical



Raman microscope WITec alpha300R

The Institute of Hydrochemistry has specialized on the analysis of MP with Raman microspectroscopy (RM) which allows an analysis down to 1 µm. Our task is to improve the existing methods for sampling, sample preparation and finally the analysis by means of RM. For sampling we will mainly focus on sediments from freshwater sources. The sample preparation will be utilized by the Munich Plastic Sediment Sepa-

rator, a system which was developed at the Institute in collaboration with the University of Bayreuth and can now be purchased commercially. For the identification of MP we will use the WITec alpha300R Raman microscope (see figure). With this system we plan to further decrease the acquisition time and improve the efficiency of RM analysis. *P. M. Anger* 

# **Evaluation of the Macro- and Microplastic Load in Freshwater Sediment Samples by means of Spectroscopic Techniques**

#### Funding: IWC

(Micro)Plastic (< 5 mm, MP) in the aquatic environment is a topic that has increasingly gained attention from the public and the scientific world over the last years. Due to its mostly higher density compared to water, plastic is to a great extent accumulated in the sediment. One can distinguish different sources of plastic in the environment. Primary MP depicts industrially produced particles, which are either directly used as product (e. g. blasting abrasives) or are utilized as additive in cosmetics or cleaning agents (e.g. peeling). Secondary MP is described as fragments or fibres, which are formed by degradation of bigger plastic parts, hence fibres from the washing of clothes are subsumed as well. Poorly managed landfills are also counting as a source for secondary MP. In wastewater treatment plants MP particles cannot be completely eliminated, that is why there is presumably remarkable, continuous а discharge into the waterbodies.

Until now it is not clear which threats are posed by MP, which is probably transferred by the food chain and transported by other media e.g. air and water to humans. Concerning the toxicity of MP for animals several effects are known, e.g. it causes cytotoxic and inflammatory responses and leads to a reduced size and population growth. This has been shown for Daphnia, rats and other model organisms. Hence effects on humans are thinkable via biomagnification.

In a recent study macroplastic (> 5 mm) was collected at two different locations on

the beaches of two lakes and at seven selected sites each at two rivers. The particles were identified by means of Infrared (IR) spectroscopy.

Furthermore, we took sediment samples at a river, up- and downstream of a wastewater treatment plant. The samples are



Photo of a macroplastic particle collected at a lake

prepared by density separation utilizing the Munich Plastic Sediment Separator to enable the analysis of the MP burden by means of Raman microspectroscopy (RM). With this method particles down to a size of 1  $\mu$ m can be analysed.

The preparation of environmental samples is a very time consuming process. To reduce the time effort we optimise different steps of the sample preparation, e.g. the elimination of organic material.

C.-C. Neumann, P. M. Anger, A. C. Wiesheu

# Raman Microspectroscopic Analysis of Microplastic Particles in Bivalves Samples

Funding: Bavarian State Ministry of the Environment and Consumer Protection (Bayerisches Staatsministerium für Umwelt und Verbraucherschutz) Cooperation: LfU Bavarian Environment Agency (Bayerisches Landesamt für Umwelt), Dr. J. Domogalla-Urbansky, F. Rager, H. Ferling, Dr. J. Schwaiger

In the last century plastic became a valuable material, which is used in manifold applications. The increased demand led to a rising production of synthetic polymers. However,

after use only 70% of these materials will be recycled or used for energy production. The rest is often carelessly disposed and can enter the environment via rivers and lakes. Since plastic is durable, it is supposed to accumulate the aquatic in environment over decades, where it can be disintegrated due to mechanical, photooxidative or microbiological influences. The resulting fragments are termed "microplastic (MP)" if their size is smaller than 5 mm. Most studies focused on the occurrence and uptake

which was taken up by indigenous bivalves Unio tumidus. The identification was performed by means of Raman microspectroscopy (RM). We improved and op-



Microplastic exposure of bivalves under standardized laboratory conditions at the Bavarian Environment Agency

timized the digestion procedure for bivalve tissue for consequent RM analyses.

Furthermore, purification steps were developed. Our results show that the identification of MP in tissue of bivalves using RM is feasible after digestion and further sample preparation. Moreover we could demonstrate the detection of MP in tissues of bivalves exposed under environmental conditions.

In the near future we will focus on further analyses of bivalves from different exposure scenarios as well as the

of MP in marine environments. But not only marine environments are contaminated, recent studies suggest that limnic ecosystems contain MP in considerable amounts.

The uptake of MP under lab conditions has been shown for different organisms including zooplankton, bivalves, crabs and fish. Our work focuses on the analysis of MP development of a digestion method for fish tissue. The evaluation of MP in aquatic organisms in combination with results from toxicological investigations, will help to provide a realistic estimation of the potential harm of MP on aquatic organisms.

A. C. Wiesheu, P. M. Anger

## Stable Isotope Surface-Enhanced Raman Scattering Microspectroscopy for Analysis of Microorganisms

### Funding: DFG, Helmholtz Zentrum München (Water Alliance) Cooperation: Dr. M. Elsner, Helmholtz Zentrum München, Institute of Groundwater Ecology, Germany; Prof. Dr. I. Kögel-Knabner, PD Dr. C. W. Müller, TUM, Chair of Soil Science and Institute of Advanced Study, TUM-IAS

With the discovery of stable isotopes in the beginning of the 20th century, stable isotopebased analytical methods are gaining more and more relevance in various scientific fields. Stable isotope Raman microspectroscopy (SIRM) opens the possibility to perform a nondestructive quantitative spatially-resolved analysis of various microbiological samples and offers fingerprint spectra with minimal or no water interference. This technique provides information on the chemical composition and structure of a sample as well as on the amount of stable isotope-marked substances. However, the sensitivity of Raman spectroscopy is quite limited. To overcome this shortcoming, surface-enhanced Raman scattering (SERS) is applied. When nanometer-sized metallic structures (Ag or Au) are brought into close contact with target molecules, electromagnetic and chemical enhancement effects can increase the Raman signal by a factor of up to 10<sup>11</sup>. However, the interpretation of the vibrational features of bacteria at the molecular level is a difficult task, since various organic substances can contribute to the SERS spectra.

In this project E. coli was used as a model organism to explore the possibilities of SERS in combination with stable isotopes (<sup>13</sup>C- and <sup>15</sup>N-labeled compounds) at single cell level and to understand the origin of certain bands in the SERS spectra. The SERS analysis of bacteria cultivated with <sup>12</sup>C-, <sup>13</sup>C- and <sup>15</sup>Ncompounds showed a very good reproducibility. Notably, a very sharp marker band at 733 cm<sup>-1</sup> for <sup>12</sup>C-microorganisms could be found. This band is significantly red-shifted to 720 cm<sup>-1</sup>, to 717 cm<sup>-1</sup>, and to 707 cm<sup>-1</sup> for <sup>13</sup>C-, <sup>15</sup>N-, and <sup>13</sup>C<sup>15</sup>N-labeled bacterial cells, respectively. With the help of the different labels the pronounced SERS band at 733 cm<sup>-1</sup> could successfully be assigned to adenine-related compounds. This result demonstrates the unique ability of the stable isotope labeling approach to understand certain spectral features in the SERS spectra of microorganisms and enables a direct comparisonof cells with different stable isotope labels.

P. Kubryk, N. P. Ivleva





SERS spectra of *E. coli* cells containing <sup>12</sup>C, <sup>13</sup>C, <sup>15</sup>N and <sup>13</sup>C<sup>15</sup>N with the red-shift of the adeninerelated marker band for stable isotope labeled samples (Kubryk et al., Analyst 2016)

### **Biomagnetic Interfaces for Non-invasive Molecular Control**

Funding: International Graduate School for Science and Engineering, IGSSE, Project BIOMAG Cooperation: Prof. Dr. G. Westmeyer, C. Massner, S. Pettinger, Chair of Biological Imaging, TUM

Among various iron oxides, Magnetite ( $Fe_3O_4$ ) and Maghemite ( $\gamma$ - $Fe_2O_3$ ) are of great interest in many biological and medical applications such as cell tracking and medical imaging due to their superparamagnetic properties. However, most current methods rely on cells with chemically synthesized magnetic nanoparticles, and potentially poor biocompatibility. Therefore, natural iron containing



Raman spectra of Ferrihydrite (black), Maghemite from commercial magnetic iron nanoparticles (blue), and Magnetite (brown)

substances in cells or proteins such as the iron-storage protein Ferritin are of great interest. However, native Ferritin shows a weak contrast in MRI because its iron core consists mainly of Ferrihydrite ( $Fe_2O_3 \cdot 0.5 H_2O$ ) which has no magnetic properties at all.

In order to increase the MRI contrast, the iron core has to be reconstituted and filled with highly magnetic iron oxides. A simple technique is available to incorporate iron oxides into the protein core of human Apoferritin. For a detailed characterization of the modified protein Raman microspectroscopy (RM) can be applied. This non-destructive analytical method is based on the effect of inelastic light scattering and provides spectra which are unique to each specific compound and therefore, provides information on its chemical composition and structure. Measurements of biological samples can be carried out with samples embedded in their natural matrix, since water is only a weak Raman scatterer.

Many iron oxides and oxyhydroxides have already been studied using RM, but there are some disagreements in the reported data. For instance, if the material such as Ferrihydrite is poorly crystallized, which is typical for environmental samples, a broadening of the bands is caused. Maghemite and Ferrihydrite have strong similarities in their Raman spectral signature. Although Maghemite bands are not well defined and the spectral signature seems to depend on sample preparation or sort of precursor because it is directly related to the degree of crystallinity of the material, it can generally be characterized by a strong broad band with two maxima around 700 cm<sup>-1</sup> and two broad bands around 380 and 500 cm<sup>-1</sup> with approximately similar intensities. Ferrihydrite, however, seems to have a strong band around 715 cm<sup>-1</sup> and two weak bands around 510 and 350 cm<sup>-1</sup>. In contrast, Magnetite shows a strong band at 665 cm<sup>-1</sup>. By comparing the Raman data and also due to the magnetic properties and biological aspects we currently assume that the iron core of Magnetoferritin consists of a mixture of different iron compounds.

C. Hartmann

## Raman Microspectroscopy for Non-invasive Threedimensional Analysis

Funding: Helmholtz Zentrum München, Water Alliance, DFG (Deutsche Forschungsgemeinschaft)

Microbes occur in their natural habitat as complex communities. In aquatic environments these tend to form cohesive structures called biofilms. A technique for the direct analysis of biofilms is essential as it was shown that microorganisms may exhibit in vitro deviating properties. In order to study the versatile interactions of prokaryotes among each other or with eukaryotic microorganisms, analytical methods with a high spatial resolution are required. Raman microspectroscopy (RM) allows to visualize microscopic structures in transparent samples three-dimensional in accordance with its chemical composition. Biofilms are highly hydrated and sensitive for external conditions. RM is well suited for the characterization of this complex ecosystem because it is a non-invasive technique with little need for sample preparations and no disturbing interference of water. Especially the ability to detect the incorporation of stable isotopes due to the resulting redshift in the position of Raman bands may provide a better understanding of processes occurring in biofilms. To cope with the small cross section of the Raman scattering, the surface-enhanced Raman spectroscopy (SERS) can be applied. The Raman signal of substances in close vicinity to metallic nanostructures is enhanced by several orders of magnitude. The figure shows the 3D SERS map of Escherichia coli cells inside of an agarose gel ( $\lambda_0 = 633$  nm, Olympus LUMPlanFI  $100\times$ , NA = 1.0). Each sphere represents the intensity of the characteristic SERS signal at

733 cm<sup>-1</sup> for the corresponding coordinate. Next to the possible detection of <sup>13</sup>C or <sup>15</sup>N with the redshift of this SERS peak, the fluorescence quenching effect of SERS implies the advantage of this procedure for the analysis of biofilms. A major aim of this





project is to evaluate the potential of 3D RM for biofilms contaminated with *L. pneumophila* which are the pathogen causing Legionnaires' disease. It is well known that *Legionella* may survive and multiply inside of several eukaryotic microbes. Even an increased virulence of intracellular *L. pneumophila* in ubiquitous amoeba is reported. With the high spatial resolution and ability to determine the uptake of stable isotopes 3D RM might prove as a useful tool for the investigation of biofilm formation in engineered water systems.

# Raman Analysis of Soil Organic Matter for Improving the Water Holding Capacity

Funding: TUM International Graduate School of Science and Engineering (IGSSE) Cooperation: Prof. Dr. I. Kögel-Knabner, Chair of Soil Science, TUM, R. Brejcha, Dr. M. Elsner, Helmholtz-Zentrum München

Due to climate change the weather conditions will alter. In future less frequent rainfall events with higher intensities have to be expected. In order to ensure constant agricultural yields, it is therefore important for the soil to store as much water as possible.



Fitted Raman spectra of a fully <sup>12</sup>C and <sup>13</sup>C labelled humic acid from 1400 to 1650 cm<sup>-1</sup>. A clear redshift of the maxima around 1600 cm<sup>-1</sup> can be seen. Inset: Raman Spectra from 1000 to 1800 cm<sup>-1</sup>.

Moreover the soil should allow the plant roots to penetrate the ground and withdraw the water when needed. A property which describes the ability of storing water in soil is the available water content (AWC). Recent studies report on a link between the amount of soil organic matter (SOM) and the AWC. Especially after adding already degraded carbon sources (e.g. biochar), an increase in the water holding capacity could be observed. The underlying mechanism, however, is not fully understood up to now.

Therefore, we introduced Raman microspectroscopy in combination with stable isotope methods (SIRM) for the analysis of SOM. In contrast to current state-of-the-art methods SIRM allows a non-destructive analysis with a spatial resolution down to 1  $\mu$ m with only low interference of water. The higher mass of the <sup>13</sup>C isotope will result in a shift to higher wavenumbers in the SIRM spectra (redshift). Since humic acids are a main component of SOM, those were used as model substances and synthesized with different isotopic ratios.

approximate relationship The linear between <sup>13</sup>C/C<sub>total</sub> ratio and the red-shift in SIRM spectra could be confirmed after optimization of the analysis methods. It was found that a controlled burning of the impurities by means of a high laser power led to the best results. The combination with Isotope-Ratio Mass Spectrometry (IR-MS) helped to validate the SIRM results and improve the limit of detection. A comparison to nano-scale Secondary Ion Mass Spectrometry (nanoSIMS) showed the potential of SIRM for the analysis of isotopically-marked SOM.

A. C. Wiesheu

## **Bioseparation and Microarray Technology (PD Dr. M. Seidel)**

## Magnetic Nanocomposites for Rapid Biosensing of Staphylococcal Enterotoxins (SET) in Complex Food Matrices

Funding: BMBF (Federal Ministry for Education and Research; Project LEVERA) Cooperation: Chair of Hygiene and Technology of Milk, LMU Munich; Institute of Veterinary Food Science, JLU Gießen; R-Biopharm AG (Darmstadt)

The aim of the project is to rapidly identify contaminations in the food supply chain and to develop fast and multiplexed analytical methods to provide a rapid diagnosis and identification of Staphylococcal enterotoxins (SET). SET are one of the most common causes of acute food poisoning, accounting for numerous foodborne-disease outbreaks all over the world.

To ensure a fast surveillance and response to foodborne-disease outbreaks, a rapid method is required which enables a sensitive quantification of proteotoxins in large volumes of complex food matrices. The inline-coupling of a facile and efficient immunomagnetic separation step based on nanocomposites with specifically tailored magnetic and morphological characteristics to a sensitive microarray analysis is a promising tool. For the detection of SET, polyclonal and monoclonal antibodies were used. The research on new antibodies was carried out by our project partner (LMU Munich and JLU Gießen). A novel synthesis approach of raspberry-shaped superparamagnetic iron oxide-shell silica-core nanocomposites was developed. Magnetic nanocomposites were fully characterized by various techniques (TEM, SEM, FT-IR, SQUID magnetometry, DLS, Raman and Moessbauer spectroscopy). The chemical longtermstability of the nanocomposites over several months was verified by Raman microspectroscopy. After the functionalization of these magnetic nanocomposites with specific detection antibodies (Ab), immunomagnetic separation (IMS) of proteotoxins directly in large volumes of food matrix is feasible. For a sensitive quantification of proteotoxins,



Schematic of the magnetic nanocomposite-based SMIA

IMS was inline-coupled with a chemiluminescence sandwich microarray immunoassay (CL-SMIA). An efficient magnetic separation was performed in 100 ml milk. A SMIA for the detection of SEB in milk was established on the flow-based microarray platform MCR 3 with a detection limit of 0.08  $\mu$ g/L. In a proof-of-concept study it was shown that SEB in milk could be successfully detected by the IMS coupled to CL-SMIA. *A. Nistler* 

# Microreactor with Integrated Characterization for the Synthesis of Magnetic Nanoparticles (MiCSMaP)

Funding: TUM International Graduate School for Science and Engineering (IGSSE) Cooperation: Dr.-Ing. B. Gleich, TUM Munich School of Bioengineering, TUM

To establish magnetic nanoparticles in the biomedical field, a high monodispersity and magnetization is of great importance. Therefore, a reproducible synthesis protocol with methods for online-characterization of magnetic nanoparticles is necessary. The MiCSMaP project focuses on the synthesis of magnetic nanoparticles and nano-



Quantification of different sized Fe nanoparticle clusters

composites in a microreactor and to couple the synthesis process with miniaturized analytical devices. This innovative system is developed together with the Munich School of Bioengineering for the determination of particle size by DLS, surface charge by measurement of the zeta-potential and relaxivity using NMR.

Magnetic nanoparticles are synthesized by a co-precipitation reaction by 3D hydrodynamic focusing of an iron salt precursor solution into a basic stream and stabilized by citrate coordination. In this way, the formation of the particles is confined to the center of the reaction channel to minimize wall effects and reactor fouling and achieve homogenous residence times and narrow size distributions. The microfluidic reactors are fabricated in-house by a cost-effective approach of using double-sided adhesive tapes and polymer films to form the microfluidic channels. 3D channel-structures can be achieved, by stacking of several tapes. The tapes are worked with a digital cutting plotter and a laser cutter, allowing for easy design adaption and fast processing.

By variation of flowrates and iron precursor concentrations, magnetic nanoparticles at defined particle and cluster-sizes could be synthesized at narrow size distributions. The  $T_2$  relaxation times of the synthesized particles were measured with the developed miniaturized NMR device to determine the relaxivities. Both, primary particle and cluster size influenced the relaxivity.

The microreactor and analysis systems are combined into one machine with integrated pumps and sample handling. The multi-step synthesis process, including the coating of the particles, can thus be monitored. In this way, quality control and online feedback is possible and synthesis parameters can be efficiently optimized to adjust the size as well as surface- and magnetic characteristics of the nanoparticles to their final application. *J. Bemetz* 

# Culture-Independent Serotyping of *L. pneumophila* in Water, Aerosol, and Urine Samples

Funding: BMBF (Federal Ministry for Education and Research; Project LegioTyper) Cooperation: Technical University of Dresden, Dresden (TUD); Bayerisches Landesamt für Gesundheit und Lebensmittelsicherheit, Erlangen (LGL); GWK Präzisionstechnik GmbH, München

Increasing numbers of legionellosis outbreaks within the last years have shown that a fast and sensitive detection method for *Legionellae* in water (e.g. surface water, drinking water, process water) and patient's urine is still needed. The gold standard for the detection of *Legionella* is the culture be defined for every serogroup and subtype of *L. pneumophila* with help of a binary code, which declares '1' above and '0' below the threshold value. In implication a pattern definition can be realised to directly and rapidly compare patient's urine samples with environmental water samples that are



Schematic of a sandwich microarray immunoassay for the monoclonal subtyping of L. pneumophila

method, which takes 10 days. However, the rapid assignment from the infected patients to the outbreak source is fundamental in case of an epidemic outbreak. Therefore, a chemiluminescence sandwich microarray immunoassay (CL-SMIA) for the detection and serotyping of Legionella pneumophila was established on the microarray analysis platform MCR-R. Within only 40 min a rapid and multiplexed detection method for serotyping of all serogroups and subtypes of L. pneumophila with a panel of 23 sensitive and selective monoclonal antibodies will be possible. For characterisation of all immobilized components a threshold value will be defined for every monoclonal antibody. A particular and unique pattern will

assumed to be the outbreak source. An application in clinical diagnostics and environmental hygiene of the health authorities is possible as the CL-SMIA is used for water samples as well as patient's urine samples. First experiments, using a new polycarbonate foil as microarray carrier, showed positive results for the detection and serotyping of *L. pneumophila* SG 1.

C. Kober, J. Bemetz

# **Concentration and Detection of Waterborne Pathogens for the Inline-Monitoring of Drinking and Raw Water**

Funding: BMBF (Federal Ministry for Education and Research; Project EDIT) Cooperation: Helmholtz-Zentrums für Umweltforschung GmbH; Institut für Mikrosystemtechnik, Universität Freiburg (IMTEK); DVGW-Technologiezentrum Wasser Karlsruhe (TZW); R-Biopharm AG (Darmstadt); GWK Präzisionstechnik GmbH (München); Fraunhofer Anwendungszentrum Systemtechnik (Ilmenau); Berliner Wasserbetriebe (BWB)

The state-of-the-art methodology to control the microbial water safety is based on periodically sampling of drinking water and quantification of to quantify indicator bacteria by cultivation and enumeration. Despite its



Automated setup for the concentration of 1 m<sup>3</sup>-water samples to a few milliliters by ultrafiltration (left) and monolithic adsorption filtration (right).

proven reliability, this approach has the disadvantages of being relatively slow and limited to a small number of indicator bacteria. The BMBF project EDIT has the aim to establish an innovative monitoring system for drinking water hygiene that combines rapid concentration methods with multiplex detection of pathogenic bacteria and viruses for on-line hygiene monitoring in waterworks. Our group has developed an ultrafiltration system that is able concentrate 1 m<sup>3</sup> of water

in less than one hour. Particles larger than 50 nm are retained. The concentrated suspension containing all microorganisms and viruses is backflushed from the ultrafiltration module and eluted for subsequent monolithic adsorption concentration by filtration (MAF). MAF discs are functionalized by anion-cation-exchanging groups to adsorb diverse bacteria and viruses in one step. Finally, a 1 mL concentrate is obtained by centrifugal ultrafiltration. After DNA or RNA extraction, the nucleic acids of bacteria and viruses are amplified under isothermal conditions on DNA microarrays at the Munich Chip Reader (MCR 3). Therefore, the recombinase polymerase amplification was implemented for flow-based chemiluminescence DNA microarrays named on-chip RPA. All systems were combined to create the hygiene-online-monitoring system (HOLM). For field tests, we have spiked bacteriophage PhiX 174 in a 40 m water line that is processed at a flow rate of 1.2  $m^3/h$ . It was shown that at least a concentration of 10<sup>6</sup> bacteriophage PhiX 174 per 10 L can be recovered by HOLM. The increased sensitivity and broader range of microbiological parameters emphasizes the need for a reconsideration of the currently used criteria for the assessment of (drinking) water hygiene.

D. Elsäßer, A. Kunze

# Regenerable Receptor-based Chemiluminescence Microarray for the Detection of Tetracycline in Liquid Samples

#### Funding: Hanns-Seidel-Stiftung

Antibiotics are widely used in animal husbandry to fight infections. As antibiotics cause dangerous resistances of bacteria, it is advisable to monitor and control the spreading of these pharmaceuticals, and to quantify them at the level of interest (maximum residue limit, if existing). Relevant materials that commonly enter the ecosystem or the food chain without any pretreatment for degradation of the antibiotics are manure that can be washed into surface waters and animal products. Therefore, a fast and cost-effective multi-analyte screening method for the monitoring of both animal products (e.g. milk) and surface waters is required.

By means of the automated flow-through analysis platform MCR 3 (GWK Präzisionstechnik, Munich), we have already established a regenerable chemiluminescence microarray immunochip for the simultaneous detection of 13 antibiotics in milk. However, the development of a regenerable immunoassay for the detection of tetracycline (one of the most frequently used antibiotics in veterinary medicine) has not been successful yet.

For this reason, a regenerable receptorbased assay according to the bacterial resistance mechanism against tetracycline is developed. A specific double-stranded DNA operator sequence TetO that may bind to the tetracycline repressor protein TetR is immobilized on the microarray surface. Biotinylated TetR is pre-incubated with the sample. The contained tetracycline binds to TetR molecules which undergo a conformational change that inhibits TetR to bind to TetO. The remaining free TetR binds to TetO and is marked with streptavidin-HRP. The higher the tetracycline concentration in the sample, the lower the intensity of the HRP-catalyzed chemiluminescence reaction.



Assessment of antibiotics in environmental matrices

This assay allows the detection of low concentrations (1 - 10  $\mu$ g/L) and the immobilized DNA double strand can be regenerated for several measurements.

The results obtained with the multianalyte microarray screening chip are to be confirmed by HPLC-MS. For this purpose, we have successfully established an HPLC-MS method that allows the detection of all the antibiotics of interest in a single run. *V. Meyer* 

# Analysis of Viruses and Antibiotic Resistant Bacteria in Irrigation Water by DNA Microarrays

Funding: BMBF (Federal Ministry for Education and Research; Project METAWATER) Cooperation: Universitat de Barcelona (Barcelona, Spain), Universitat Politecnica de Valencia (Valencia, Spain), Universitat Rovira I Virgil (Tarragona, Spain), Bayerische Landesamt für Gesundheit und Lebensmittelsicherheit (LGL), State General Laboratory (Cyprus), Technical University of Denmark (Copenhagen, Denmark)

An increasing number of epidemic outbreaks is associated with the consumption of fruits and vegetables. Due to the World Health Organization (WHO) a reasonable explanation could be the irrigation with contaminated water. Depending on its origin irrigation water could contain a high amount of micro-



Schematic of the DNA microarrays

biological and viral contaminants with only a low number of pathogens. To date, there is no European guideline defining quality standards for irrigation water. To protect consumer's health as well as to ensure the production of safe food, screening, monitoring and controlling of microbiological hazard in irrigation water are highly needed.

Pathogens in water used for irrigation (surface and groundwater) are concentrated by monolithic affinity filtration (MAF). Bacteria and viruses are identified by species-specific genes via qPCR and DNA microarray. DNA microarray experiments are performed on the MCR 3 platform. In contrast to conventional methods based on cultivation, DNA microarrays enable a fast and multiplex analysis of different pathogens at the same time.

During the project, theme-related DNA microarrays will be synthesized. These arrays detection concern the of emergent pathogens, ESBL-producing bacteria as well as the trace back of fecal contaminations. To achieve an European scale identification, experimental protocols for pathogen concentration and quantification were harmonized in all partner laboratories. We performed an European proficiency test together with our partner laboratories of Spain and Denmark. In this experiment we compared our MAF with skimmed-milk flocculation (SMF), another concentration method established at our Spanish partner laboratory. Therefore, we distributed aliquots different concentrations of containing viruses partner bacteria and to our laboratories, which were spiked into 10 L mineral water, concentrated and quantified. Independently of the laboratory, it was shown that MAF has a higher capacity of recovering viruses even at low concentrations compared to SMF. During the experimental procedure and data analysis we furthermore evaluated crucial steps of an European proficiency test to optimize future experiments.

S. Schäfer

# Aerosol Research (Prof. Dr. R. Niessner)

# **Bioaerosol Chamber for Legionella Containing Shower Aerosols**

Funding: Bayerisches Landesamt für Gesundheit und Lebensmittelsicherheit (LGL) Cooperation: LGL, TU Dresden, Prof. Lück

A bioaerosol chamber for a targeted generation of Legionella containing shower aerosols was developed in a project funded by the Bavarian Health and Food Safety Authority. Until now, the risk assessment of shower bioaerosols was only considered by exposition models. The lack of bioaerosol shower chambers with which pathogenic Legionella spp. in showers could be handled was one reason. Legionella spp. are classified as biosafety level 2. Therefore, a bioaerosol shower chamber was integrated in a biosafety cabinet according to the chamberin-chamber-principle. Thereby the biosafety cabinet works under negative pressure. Shower bioaerosols were generated in the

bioaerosol chamber and directly collected by impingement using the sampling head of Coriolis µ in the biosafety cabinet. We found that 0.0006% of E. coli spiked in tap water were recovered in bioaerosols during our experiments. The system is now ready for further experiments with Legionella pneumophila. Experimental data of bioaerosol size distributions, the partitioning of the distribution of Legionella spp. from tap water into shower aerosols as well as the microbiological activity are important to improve the risk analysis of legionella containing shower aerosols.

B. Kiwull, A. Wunderlich, M. Seidel



**Bioaerosol Chamber** 

## Particle behavior in Ranque-Hilsch Vortex Tubes (RHVT)

Funding: IWC

The Ranque-Hilsch Vortex Tube (RHVT), First described by J.-G. Ranque in 1933 and rediscovered, improved, and modified by R. Hilsch (1946) has primarily attracted attention because of its ability to produce temperature differences in a split gas flow.

A RHVT consists of a main tube connected to a vortex chamber, having a tangentially oriented inlet nozzle. When a



Schematic drawing of a Ranque-Hilsch vortex tube (Liew et al, Phys. Rev. Lett. 109, 054503, 2012)

pressurized gas is injected tangentially a strong rotational flow field is generated. This swirl flow propagates till the end of the main tube where a defined fraction of gas leaves the device through a valve at a higher temperature than at the inlet. However, it is observed that two vortices occur inside the tube, one at the periphery of the tube and the other at the core of the tube with opposite flow direction (see figure). While the external flow exits at the hot outlet the counter flow exits at the cold orifice with a temperature much lower than the inlet temperature.

The underlying physical processes that determine the temperature separation have

not been resolved completely in the past. Numerous theories, which explain the energy separation process are given in literature. Research on vortex tube generally focuses on the following aspects: the three-dimensional distributions of tangential velocities, compressible fluid dynamics of turbulent flow, thermodynamics, and heat transfer. These aspects make the research complicated and challenging.

However, C. U. Linderstrom-Lang reported in 1964 (Int. J. Heat Mass Transfer, 7, 1195-1206) that RHVTs may act as separators of gas mixtures. The author concludes, though in some cases from rather inaccurate data, that gas mixture separation does take place. Further, several authors report on the RHVT as a mass separation device, but no experimental data have been published so far.

Therefore, experimental studies of a laboratory RHVT device could gain important new insight. Geometrical and thermophysical parameters of a RHVT are investigated in order to implement thermal separation processes in a mathematical model, which already now shows good consistency with experimental data. The behavior of nanometer-sized particles in the RHVT is studied by measuring injected particle concentrations using a SMPS. A further goal is to predict the particle behavior by mathematical modeling.

F. Hagen, C. Haisch

## The Catalytic Effect of Potassium Compounds on Soot Oxidation

#### Funding: IWC

Cooperation: Ultramicroscopy Research Center at Kyushu University, Fukuoka (Japan)

Diesel soot is one of the major pollutants in the world and is classified as carcinogenic. Soot/black carbon also has the second largest impact on global warming after CO<sub>2</sub>. In North America and Europe, soot is mainly emitted by diesel engines, which are mostly equipped with particulate filters to minimize emissions. Regeneration of these filters is done by oxidation (combustion) of the soot. Uncatalyzed oxidation requires temperatures > 600 °C in O2, which result in poor fuel efficiencies. Additives can enhance soot reactivities during soot formation, leading to internally-mixed soot and possible oxidation temperatures under 400 °C. Besides oxides, also salts are able to lower the temperatures for soot oxidation significantly. Nevertheless, research towards a more comprehensive understanding of combustion is still needed.

Therefore, different soot, internally-mixed with potassium salts, were produced using a custom-built diffusion burner and collected thermophoretically or on quartz fiber filters. The soot were studied regarding their salt content (atomic absorption spectroscopy, AAS), their oxidation reactivity (temperatureprogrammed oxidation, TPO), their structural parameters (Raman microspectroscopy, BET analysis, scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM)) as well as their electronic structure using electron paramagnetic resonance spectroscopy (EPR). Soot aerosols were also characterized regarding their particle number concentrations using a scanning mobility particle sizer (SMPS) setup.

All salts lead to a marked decrease of the TPO temperature of maximum  $CO + CO_2$  emissions ( $T_{max}$ ) with  $K_2CO_3$  leading to a decrease of up to 300 °C compared to uncatalyzed soot. Increased salt-contents also lead to lower ratios of  $CO/CO_2$  at  $T_{max}$ . Structural parameters of the different soot derived from Raman Microspectroscopy, SEM and SMPS did not vary significantly compared to uncatalyzed soot, BET areas only showed slight trends.

In contrast, the oxidation reactivity could be correlated to parameters derived from HRTEM and EPR measurements. The results show the catalytic potential of potassium compounds and give new indications towards a more complete understanding of the catalyzed soot oxidation. They also show the need for a fast and on-line method to fully characterize soot oxidation reactivity, which is currently under development. *A. Rinkenburger* 



Contour plot of T<sub>max</sub> (TPO) vs. BET areas and soot salt content.

# **Publications**

## **Peer Reviewed Journals**

- M. Ben Haddada, M. Huebner, S. Casale, D. Knopp, R. Niessner, M. Salmain and S. Boujday; Gold Nanoparticles Assembly on Silicon and Gold Surfaces: Mechanism, Stability and Efficiency in Diclofenac Biosensing. J. Phys. Chem. C 120 (2016) 29302-29311
- M. N. Ess, M. Bürger, W. Mühlbauer, S.I. Seher, Untersuchung der Rußreaktivität unterschiedlicher Dieselkraftstoffe, MTZ Motortechnische Zeitschrift 77 (2016) 70-78.
- M. N. Ess, M. Bürger, W. Mühlbauer, S.I. Seher, Examination of the Soot Reactivity of Different Diesel Fuels, MTZ worldwide 77 (2016) 66-71.
- M. N. Ess, H. Bladt, W. Mühlbauer, S. Seher, C. Zöllner, S. Lorenz, D. Brüggemann, M. Nieken,
  N. Ivleva and R. Niessner; Reactivity and Structure of Soot Generated at Varying Biofuel
  Content and Engine Parameters. Combust. Flame 163 (2016) 157-169
- M. N. Ess, D. Ferry, E. Kireeva, R. Niessner, F.-X. Ouf and N. Ivleva; In Situ Microspectroscopy Analysis of Soot Samples with Different Organic: Structural Changes During Heating. Carbon 105 (2016) 572-585
- M. Göttel, R. Niessner, N. Pluym, G. Scherer and M. Scherer; A Fully Validated GC-TOF-MS Method for the Metabolic Profiling of Fatly Acids in Human Plasma. J. Chromatogr. B 1041/1042 (2016) 141-150
- A. Hlavacek, Z. Farka, M. Hübner, V. Hornakova, D. Nemecek, R. Niessner, P. Skladal, D. Knopp and H. H. Gorris; A Competitive Upconversion-linked Immunosorbent Assay (ULISA) for the Rapid and Sensitive Detection of Diclofenac. Anal. Chem. 88 (2016) 6011-6017
- J. Ho; M. Seidel; R. Niessner; J. Eggers and A. Tiehm; Long Amplicon (LA)-qPCR for the Discrimination of Infectious and Noninfectious X174 Bacteriophages After UV Inactivation. Water Res. 103 (2016) 141-148
- H. Imhof, C. Laforsch, A. Wiesheu, J. Schmid, P. Anger, R. Niessner and N. Ivleva; Pigments and Plastic in Limnetic Ecosystems: A Qualitative and Quantitative Study on Microparticles of Different Size Classes. Water Res. 98 (2016) 64-74
- N. P. Ivleva, A. C. Wiesheu & R. Niessner; Microplastik in aquatischen Ökosystemen. Angew. Chemie German Edition (2016) DOI: 10.1002/ange.201606957
- N. P. Ivleva, A. C. Wiesheu & R. Niessner; Microplastic in Aquatic Ecosystems. Angew. Chemie Intern. Edition (2016) DOI: 10.1002/anie.201606957
- D. Karthe, O. Behrmann, V. Blättel, D. Elsässer, C. Heese, M. Hügle, F. Hufert, A. Kunze, R. Niessner, J. Otto, B. Scharaw, M. Spoo, A. Tiehm, G. Urban, S. Vosseler, T. Westerhoff, G. Dame and M. Seidel; Modular Development of an Inline Monitoring System for Waterborne Pathogens in Raw and Drinking Water. Environ. Earth Sciences 75 (2016) 1481, 16 pages
- B. Kiwull, A. Wunderlich, R. Niessner, M. Seidel and C. Herr; Bioaerosol Chamber for Legionella Containing Shower Aerosols. Gefahrstoffe-Reinhaltung der Luft 76 (2016) 344-350

- P. Kubryk, R. Niessner and N. Ivleva; On the Origin of the Band at around 730 cm-1 in SERS Spectra of Bacteria: Stable Isotope Approach. Analyst 141 (2016) 2874-2878
- A. Kunze, M. Dilcher, A. Abd el Wahed, F. Hufert, R. Niessner and M. Seidel; On-chip Isothermal Amplification on Flow-based Chemiluminescence Microarray Analysis Platform for the Detection of Viruses and Bacteria. Anal. Chem. 88 (2016) 898-905
- Y. Lin, Q. Zhou, D. Tang, R. Niessner, H. Yang and D. Knopp; Silver Nanolabels-Assisted Ion-Exchange Reaction with CdTe Quantum Dots Mediated Exciton Trapping for Signal-On Photoelectrochemical Immunoassay of Mycotoxins. Anal. Chem. 88 (2016) 7858-7866
- V. Meyer, D. Meloni, F. Olivo, E. Märtlbauer, R. Dietrich, R. Niessner and M. Seidel; Validation Procedure for Multiplex Antibiotic Immunoassays Using Flow-based Chemiluminescence Microarrays. In: Methods in Molecular Biology, Small Molecule Microarrays: Methods and Protocolls, edited by S. Q. Yao and M. Uttamchandani, Springer, Heidelberg 1518 (2017) 195-212
- A.-C. Neumann, X. Wang, R. Niessner and D. Knopp; Determination of Microcystin-LR in Surface Water by a Magnetic Bead-based Colorimetric Immunoassay Using Antibodyconjugated Gold Nanoparticles. Anal. Meth. 8 (2016) 57-63
- G. Pang, J. Laufer, R. Niessner and C. Haisch; Photoacoustic Signal Generation in Gold Nanospheres in Aqueous Solution: Signal Generation Enhancement and Particle Diameter Effects. J. Phys. Chem. C 120 (2016) 27646-27656
- L. Pang, M. Lafogler, B. Knorr, E. McGill, D. Saunders, T. Baumann, P. Abraham & M. Close, Influence of Colloids on the Attenuation and Transport of Phosphorus in Alluvial Gravel Aquifer and Vadose Zone Media, Sci. Tot. Environ. 550 (2016) 60-68.
- J. Plank, M. Zhang-Preße, N. Ivleva and R. Niessner; Stability of Single Phase C3A Hydrates Against Pressurized CO<sub>2</sub>. Constr. & Building Mater. 122 (2016) 426-434
- S. Seher, M. N. Ess, H. Bladt, R. Niessner, G. Eigenberger and U. Nieken; A Comparison of Diesel Soot Oxidaten Rates Measured with Two Different Isothermal Set-ups. J. Aerosol Sci. 91 (2016) 94-100
- M. Seidel, L. Jurzik, I. Brettar, M. Hoefle, C. Griebler, Microbial and Viral Pathogens in Freshwater – Current Research Aspects Studied in Germany. Environ. Earth Sci. 75 (2016) 1384
- I. Sidorenko, S. Nizamov, R. Hergenröder, A. Zybin, A. Kuzmichev, B. Kiwull, R. Niessner and V. Mirsky; Detection and Quantification of Images of Single Nanoparticles in Surface Plasmon Microscopy. Microchim. Acta 183 (2016) 101-109
- M. Tschofen, D. Knopp, E. Hood, E., Stöger; Plant Molecular Farming: Much More Than Medicines. Ann. Rev. Anal. Chem. 9 (2016) 271-294
- X. Wang, R. Niessner, D. Tang and D. Knopp; Nanoparticle-based Biosensors and Immunoassays for Aflatoxins. Anal. Chim. Acta 912 (2016) 10-23
- A. Wiesheu, P. Anger, T. Baumann, R. Niessner and N. Ivleva; Raman Microspectroscopic Analysis of Fibers in Beverages. Anal. Meth. 8 (2016) 5722-5725
- A. Wunderlich, C. Torggler, D. Elsässer, C. Lück, R. Niessner and M. Seidel; Rapid Quantification Method for *Legionella Pneumophila* in Surface Water. Anal. & Bioanal. Chem. 408 (2016) 2203-2213
- Y. Ying, D. Yang, H. Zhou, C. Haisch and R. Niessner; Reproducible E. coli Detection Based on Label-free SERS and Mapping. Talanta 146 (2016) 457-463

# **Conference Presentations**

#### **Oral Presentations**

- S. Amininejad, R. Weiss, N. Ivleva, R. Niessner and T. Baumann, Visualization of Titanium Dioxide Nanoparticles in Environmental Samples by Using Raman Microspectroscopy, International Workshop on Engineered Nanoparticles in Environmental Systems: Fate, Transport, Effects and Analytics, 20.-21.10.2016, Landau/Pfalz.
- T. Baumann, Validation of Hydrochemical Analyses and Gas Concentrations of Deep Geothermal Aquifers, 41st Workshop on Geothermal Reservoir Engineering, 22.-24.2.2016, Stanford, U.S.A.
- M. N. Ess, D. Ferry, E. D. Kireeva, R. Niessner, François-Xavier Ouf and N. P. Ivleva, Comprehensive Structural Analysis of Soot Samples With Different OC Content by Means of HRTEM, FTIR Spectroscopy and Raman Microspectroscopy, European Aerosol Conference, EAC 2016, 5.-9.9.2016, Tours, France.
- M. Herbrich, B. Köhl and T. Baumann, Scalings at Geothermal Facilities Exploring the Malm Aquifer (Bavarian Molasse Basin), EGU General Assembly, 17.-22.4.2016, Vienna.
- C. Kober, A. Wunderlich, C. Herr, C. Lück, R. Nießner, M. Seidel, Culture-Independent Serotyping of *L. pneumophila* in Water, Aerosol and Urine Samples, BIODEFENSE, 26.-29.04.2016, Munich.
- M. Lafogler, F. Wenderoth, J. Bartels, G. Somogyi, T. Hinkofer, K. Hess and T. Baumann, Processes in the Vicinity of an Injection Well of a Geothermal Facility in the Malm Aquifer, 41st Workshop on Geothermal Reservoir Engineering, 22.-24.2.2016, Stanford, U.S.A.
- M. Lafogler, F. Wenderoth, J. Bartels, G. Somogyi, T. Hinkofer, K. Hess and T. Baumann, Processes in the Vicinity of an Injection Well of a Geothermal Facility in the Malm Aquifer (Bavarian Molasse Basin), 25. Tagung der FH-DGGV, 13.-17.4.2016, Karlsruhe.
- W. Mühlbauer, U. Nieken, M. N. Ess, U. Janoske, Einfluss der Rußreaktivität auf die DPF-Regeneration, Forschungsvereinigung Verbrennungskraftmaschinen e.V. Frühjahrstagung 2016, 14.04.2016, Bad Neuenahr.
- A.-C. Neumann, S. Melnik, R. Niessner, E. Stöger, D. Knopp. Quantitative Abreicherung von Cyanotoxinen aus Oberflächenwasser mittels rekombinant in Pflanzen hergestellter Antikörper (Plantibodies). Fachgruppe Wasserchemische Gesellschaft, WASSER 2016, 2.-4.5.2016, Bamberg.
- A. Nistler, M. Sandhu, R. Dietrich, E. Maertelbauer, R. Niessner, M. Seidel, Magnetic Nanocomposites for Rapid Biosensing in Complex Matrices, Biosensors 2016, 24-27.5.16, Gothenborg, Sweden.
- M. Seidel, Multiplexed On-Chip Isothermal Nucleic Acid Amplification on Flow-Based Chemiluminescence Microarrays. Biosensors 2016, 45.-27.5.2016, Gothenburg, Sweden.
- M. Seidel, New Detection Methods for *Legionella* in Water and Air. 14.3.2016, Mini-Symposium der Fachgruppe Wasser / Abwasser bei VAAM-Jahrestagung, Jena.
- M. Seidel, A, Wunderlich, B. Kiwull, B. Bartha, S. Walser, B. Brenner, S. Huber, C. Lück, C. Höller, C. Herr, R. Niessner, *Legionella* Bioaerosols – Generation, Sampling and Rapid Detection by Culture-Independent Methods. 14.-15.4.2016, AUVA Bioaerosol Chamber Expert Meeting, Vienna, Austria.
- M. Seidel, Microarray-basiertes Messverfahren zur schnellen Quantifizierung von lebenden *Legionella spp.* und *Legionella pneumophila* in Verdunstungskühlanlagen. 20.9.2016, VDI Expertenforum Legionellen aus Verdunstungsrückkühlanlagen - Aktuelle Entwicklungen, Bonn.
- M. Seidel, Schnelle Multianalytbestimmung von Bakterien und Viren im Wasser mittels DNAund Antikörper-Mikroarrays, 15.9.2016, 10. Weihenstephaner Seminar für Wassertechnologie, Freising.
- M. Seidel, Rapid Quantification of *Legionella pneumophila* on the Microarray Analysis Platform MCR 3, International Symposium on Legionella ecology, virulence and risk assessment, Helmholtz Center for Infection Research, 6.-7.9.2016, Braunschweig, Germany.
- M. Seidel, Schnelle Multianalytbestimmung von Bakterien und Viren im Wasser mittels DNAund Antikörper-Mikroarrays, 15.9.2016, 10. Weihenstephaner Seminar für Wassertechnologie, Freising.
- M. Ueckert, R. Niessner and T. Baumann, High Temperature Aquifer Storage, 41st Workshop on Geothermal Reservoir Engineering, 22.-24.2.2016, Stanford, U.S.A.
- M. Ueckert, R. Niessner and T. Baumann, High Temperature Aquifer Storage, EGU General Assembly, 17.-22.4.2016, Vienna.

## **Poster Presentations**

- P. M. Anger, A. C. Wiesheu, F. Rager, H. Ferling, J. Domogalla-Urbansky, J. Schwaiger, R. Niessner, N. P. Ivleva, Analysis of Microplastic Particles in Bivalve Samples, European Conference on Plastics in Freshwater Ecosystems, 21.-22.6.2016, Berlin, Germany.
- P. M. Anger, A. C. Wiesheu, T. Baumann, R. Niessner, N. P. Ivleva, Fibers in Beverages: Raman Microspectroscopic Analysis, Late Summer Workshop "Microplastics in the Aquatic Environments", 16.-18.6.2016, Haltern am See.
- S. Barnikol, G. Metreveli, F. Seitz, R. R. Rosenfeldt, S. K. Kumahor, A. Grün, D. Rakcheev, T. Baumann, M. Bundschuh, F. Lang, S. Klitzke, W. Manz, R. Schulz, H.-J. Vogel, G. E. Schaumann: Mesokosmos-Studie zur Charakterisierung des Verbleibs und der Wirkung synthetischer Silbernanopartikel an einer aquatisch-terrestrischen Übergangszone, WASSER 2016, , 2.-4.5.2016, Bamberg.
- T. Baumann, M. Lafogler, F. Wenderoth and J. Bartels, Processes in the Vicinity of an Injection Well of a Geothermal Facility in the Malm Aquifer, EGU General Assembly, 17.-22.4.2016, Vienna.
- L. Degenkolb, S. Klitzke, G. Metreveli, S. Kumahor, G. Schaumann, T. Baumann, H.-J. Vogel, M. Kaupenjohann, F. Lang: Remobilization of Ag NP Retained in Sediments of an Artificial Riverbank Filtration system. International Workshop on Engineered Nanoparticles in Environmental Systems: Fate, Transport, Effects and Analytics, 20.-21.10.2016, Landau/ Pfalz.
- M. N. Ess, B. Grob, N. P. Ivleva, R. Niessner, In Situ Raman Microspectroscopic Analysis of Soot During Temperature Programmed Oxidation, European Aerosol Conference 2016, 4.-9.9.2016, Tours, France (Best Poster Award).
- M. Herbrich, B. Köhl and T. Baumann, Scalings at Geothermal Facilities Exploring the Malm Aquifer in the Bavarian Molasse Basin, 25. Tagung der FH-DGGV, 13.-17.4.2016, Karlsruhe.

- B. Kiwull, A. Wunderlich, S. Walser, B. Bartha, B. Brenner, S. Huber, C. Lueck, C. Hoeller, C. Herr, M. Seidel, R. Niessner, Investigations on *Legionella* Containing Aerosols: Set-up of a Model Shower Aerosol Chamber, European Aerosol Conference 2016, 4.-9.9.2016, Tours, France.
- B. Kiwull, A. Wunderlich, S. Walser, B. Bartha, B. Brenner, S. Huber, C. Lueck, C. Hoeller, C. Herr, M. Seidel, R. Niessner, Investigations on *Legionella* Containing Aerosols: Set-up of a Model Shower Aerosol Chamber, BIODEFENSE 2016, 26.-29.4.2016, Munich.
- B. Köhl, R. Niessner and T. Baumann, Teilprojekt Scaling Prinzip, wissenschaftliche Fragestellungen und Lösungsansätze, Auftaktveranstaltung Geothermie-Allianz Bayern, 30.9.2016, Garching b. München.
- B. Köhl, R. Niessner and T. Baumann, Scalings at Geothermal Facilities Exploring the Malm Aquifer (Bavarian Molasse Basin), European Geothermal PhD-day, 24.-26.2.2016, Bari.
- B. Köhl, R. Niessner and T. Baumann, Scalings at Geothermal Facilities (Bavaria), Münchener Wissenschaftstage, 12-15.11.2016, Munich.
- C. Kober, A. Wunderlich, J. Bemetz, C. Herr, C. Lück, R. Nießner, M. Seidel, Culture-Independent Serotyping of L. Pneumophila in Water, Aerosol and Urine Samples, WASSER 2016, 2.-4.5.2016, Bamberg.
- P. Kubryk, R. Weiss, R. Niessner, N. P. Ivleva, Stable-isotope SERS Analysis of Microorganisms in Aqueous Systems, WASSER 2016, 2.-4.5.2016, Bamberg.
- G. Metreveli, S. Kurtz, F. Seitz, R. R. Rosenfeldt, A. Grün, S. K. Kumahor, T. Baumann, M. Bundschuh, F. Lang, S. Klitzke, W. Manz, R. Schulz, H.-J. Vogel, G. E. Schaumann: Fate and Effects of Engineered Silver Nanoparticles in the Aquatic-terrestrial Transition Zone: A Floodplain Mesocosm Study. 11 th International Conference on the Environmental Effects of Nanoparticles and Nanomaterials (ICEENN 2016), 14.-18.8.2016, Golden, Colorado, U.S.A.
- A. Nistler, E. Linares, R. Dietrich, E. Maertelbauer, T. Wittwer, R. Niessner, M. Seidel, Rapid and Sensitive Detection of Staphylococcal Enterotoxins by Immunomagnetic Separation Inline-Coupled Microarray Analysis, BIODEFENSE, 26.-29.4.2016, Munich.
- A. Rinkenburger and R. Niessner, Characterization of internally-mixed soot aerosols Is there a correlation between particle size, surface area and reactivity?, European Aerosol Conference 2016, 4.-9.9.2016, Tours, France.
- S. Schäfer, R. Niessner, and M. Seidel, Rapid Detection of ESBL-Producing Bacteria in Irrigation Water by DNA Microarrays, BIODEFENSE, 26.-29.4.2016, München, Germany
- M. Ueckert, R. Niessner and T. Baumann, High Temperature Aquifer Storage, 25. Tagung der FH-DGGV, 13.-17.4.2016, Karlsruhe.
- A. C. Wiesheu, F. Rager, P. M. Anger, H. Ferling, J. Domogalla-Urbansky, J. Schwaiger, R. Niessner, N. P. Ivleva, Aufschluss und Identifikation von Mikroplastik in limnischen Organismen, WASSER 2016, 2.-4.5.2016, Bamberg.

- A. C. Wiesheu, R. Nießner, N. P. Ivleva, Stabilisotopen-Raman-Mikrospektroskopie (SIRM) zur Analyse von organischen Substanzen im Boden, WASSER 2016, 2.-4.5.2016, Bamberg.
- A. C. Wiesheu, P. M. Anger, H. K. Imhof, C. Laforsch, R. Niessner, N. P. Ivleva, Qualitative and Quantitative Analysis of Microplastic and Pigment Particles in Freshwater, European Conference on Plastics in Freshwater Ecosystems, 21.-22.6.2016, Berlin, Germany.
- A. C. Wiesheu, P. M. Anger, H. K. Imhof, C. Laforsch, R. Niessner, N. P. Ivleva, Micro-sized Pigments and Plastic in Freshwater: Identification and Quantification by Raman Microspectroscopy, Late Summer Workshop "Microplastics in the Aquatic Environments", 16.-18.6.2016, Haltern am See.
- C. Wismeth, S. Muffler, M. Ueckert, R. Niessner and T. Baumann, Fluid-Matrix Interactions During High-Temperature Aquifer Storage - Lab Experiments and Modelling, 25. Tagung der FH-DGGV, 13.-17.4.2016, Karlsruhe.
- C. Wismeth, S. Muffler, M. Ueckert, R. Niessner and T. Baumann, Fluid-Matrix Interactions During High-Temperature Aquifer Storage - Lab Experiments and Modelling, EGU General Assembly, 17.-22.4.2016, Vienna.

## **Invited Lectures**

- T. Baumann, Visualization of Fluid Motion at Non-Aqueous Phase Interfaces, IMMENS Kickoff Meeting, 29.-30.9.2016, Bergen, Norway.
- T. Baumann and M. Ueckert, High Temperatature Storage in Reactive Aquifers A Hydrogeochemists Perspective, Themses Kickoff Meeting, 26.-28.9.2016, Bergen, Norway.
- T. Baumann, Nanopartikel in aquatischen Systemen Fluch und Segen, BAM Themenfeld Workshop Umwelt, 15.3.2016, Berlin.
- N. P. Ivleva, Raman Microspectroscopy and SERS for Analysis of Biofilms, Hong Kong University of Science and Technology, HKUST, 8.6.2016, Hong Kong, China.
- N. P. Ivleva, Microplastics in Aquatic Ecosystems: Focus on Raman Microspectroscopic Analysis, Karlsruhe Institute of Technology, KIT, 15.7.2016, Karlsruhe, Germany.
- N. P. Ivleva, Identification and Quantification of Microplastic in Environmental Samples, International Summer School "Microplastic in Aquatic Environment", 25.-28.9.2016, Haltern am See, Germany.
- N. P. Ivleva, Analytik von Mikroplastik in aquatischen Systemen mit spektroskopischen Verfahren, 2. Wasseranalytisches Seminar, MWAS 2016, 14.-15.9.2016, Mülheim an der Ruhr, Deutschland.
- N. P. Ivleva, Selektive Analytik von Mikroplastik mittels Raman-Mikrospektroskopie, Bund/ Länder-Gespräch "Mikroplastik in Binnengewässern", 10.3.2016, Wielenbach, Deutschland.
- N. P. Ivleva, Nachweisbarkeit von Mikroplastik in Wasserproben aktuelle Forschungsergebnisse, VBEW-Fachtagung Wasser 2016, 17.3.2016, Straubing, Deutschland.

- D.Knopp, A.-C. Neumann, S. Melnik, R. Niessner, E. Stöger. Approach to Depletion of Cyanotoxin-MC-LR From Surface Water Using Plantibody-Doped Porous Filter. 18th International Symposium on Advances in Extraction Technologies & 22nd International Symposium on Separation Sciences (ExTECH), 03.-06.07.2016, Torun, Poland.
- D. Knopp and E. Stöger. Antibodies as Highly Affine and Specific Reagents for Bioanalytical Applications – Plants as Emerging Antibody Source. The 1st International Conference on Applied Sciences (ICAS-1), 20.-21.07.2016, Ho Chi-Minh City, Vietnam.
- D. Knopp. Application of (Bio)analytical Methods for Food Safety Monitoring and Authentication – Review. Analytica Anacon India, 21.-22.10.2016, Hyderabad, India.
- R. Niessner, Characterization of Nanoparticles in Different Spheres, Institute of Advanced Studies, HKUST, Distinguished Lecture, 10.3.2016, Hong Kong.
- R. Niessner, Ways to Characterize Hydrosols, Hong Kong University of Science and Technology, Dept. of Civil Engineering, 13.3.16, Hong Kong.
- R. Niessner, Water-A Simple Compound with Past and Future, Kyushu University, Dept. of Engineering, 23.3.2016, Fukuoka
- R. Niessner, Rudolf Bock-Gedächtnisvorlesung, Analytica, 10.5.2016, München.
- R. Niessner, Sensing Technologies for Particle Characterization (Hydrosols & Aerosols), 9th Senftenberg Innovations Forum, 1. and 2.6.2016, Senftenberg.
- R. Niessner, Microarray Technologies with Antibodies, Oligonucleotides and Nanoparticles, ISEAC 39, 19.7.2016, Hamburg.
- M. Seidel, Microarray-basiertes Messverfahren zur schnellen Quantifizierung von lebenden Legionella spp. und Legionella pneumophila in Verdunstungskühlanlagen. 20.9.2016, VDI Expertenforum Legionellen aus Verdunstungsrückkühlanlagen - Aktuelle Entwicklungen, Bonn.
- M. Seidel, Rapid Concentration and Microarray-Based Detection Methods for Pathogens in Water and Food, 24.10.2016, Hahn-Schickard, Freiburg, Germany.
- A. C. Wiesheu, P. M. Anger, R. Niessner, N. P. Ivleva, Microplastic Analysis in Various Matrices – Sampling, Sample Processing and Identification, Thermo Scientific Workshop "Insights and analytical approaches on Microplastics using Raman and FTIR Spectroscopy", 31.11.2016, Dreieich, Germany.

#### Scientific Committees

- T. Baumann, Engineered Nanoparticles in Environmental Systems: Fate, Transport, Effects and Analytics 20.-21.10.2016, 2016 Landau in der Pfalz, Germany (Scientific Advisory Panel)
- T. Baumann, Fate and Transport of Biocolloids and Nanoparticles in Soil and Groundwater, EGU General Assembly, 17-22.4.2016, Vienna (Convener)
- D. Knopp, The 1st International Conference on Applied Sciences (ICAS-1), 20.-21.07.2016, Ho Chi-Minh City, Vietnam (Conference Chair)

### Hydrochemical consulting

Mineralisation control analyses: Bad Abbach, Bad Aibling, Bad Birnbach, Bad Füssing, Bad Griesbach, Bad Gögging, Bad Reichenhall, Bad Rodach, Bad Staffelstein, Bad Wiessee, Bad Wimpfen, Bad Wörishofen, Bayreuth, Erding, Hölle, Kondrau, Neumarkt i. d. Opf., Sibyllenbad, Straubing, Weißenstadt

Hydrogeological and hydrochemical expertises (mineral water, spa water): Bad Endorf, Bad Steben, Bad Wiessee, Siegsdorf

Deep Hydrogeothermal Energy Exploration: Aschheim, Freiham, Holzkirchen, Pullach, Sauerlach, Waldkraiburg



Piper diagram of the analyses performed in 2016

## Theses

## PhD Theses

- MSc Chem. Michaela Eß: Oxidationsreaktivitätsbestimmung und Strukturanalyse von Propanrußen und motorischen (Bio) Dieselrußen
- Dipl. Ing. Chem. Moritz Herbrich: Facility and Safety Related Processes in the Thermal Water Cycle of a Geothermal Heat and Power Station
- MSc Chem. Andreas Kunze: Aufkonzentrierung und Detektion viraler und bakterieller Pathogene in Trinkwasser
- MSc Chem. Anna Catherine Neumann: Entwicklung eines Abreicherungsverfahrens für Microcystin-LR aus Wasserproben mit rekombinant in Pflanzen hergestellten Antikörpern (Plantibodies)
- MSc Chem. Christian Metz: Gasblasenbildung und Sorption von organischen SERS-aktiven Substanzen an mikro-und nanostrukturierten Oberflächen
- MSc Geo. Martina Ueckert: Hochtemperaturaquiferspeicher in den Malmcarbonaten des bayerischen Molassebeckens

#### M.Sc. Theses

- BSc Philipp Anger: Raman Microspectroscopic Analysis of Microplastic in Environmental Samples
- BSc Nadine Berger: Immunoassay based on Decoding Magnetic Nanoparticles for the Detection of Staphylococcus Enterotoxins
- Cand. Staats. Exam. Sebastian Dirndorfer: Entwicklung immunologischer Teststreifen für den Nachweis von Diclofenac und Microcystin-LR unter Verwendung von murinen Antikörpern und Plantibodies
- BSc Selina Muffler: Hydrogeochemische Simulation eines Hochtemperatur-Aquiferspeichers im Malm-Aquifer
- BSc Laura Sanchez: Quantification of Anitbiotics in Environmental Water and Milk Samples by a Combination of Monolithic Disks and Liquid Chromatography-high resolution Mass Spectrometry
- BSc Veronika Stiegler: Immobilization of Antibiotics on Monolithic Columns to Concentrate Gram-negative and Gram-positive Bacteria from Fluids
- BSc Carina Wismeth: Autoclave Experiments with Core Samples to Quantify the Matrix Interaction and the Stability of the Matrix During Injection and with Drawal Cycles

### **B.Sc.** Theses

- Christian Biermaier: Synthesis and Characterisation of a Functional Coating on Polycarbonatefoil for the Application in Microarray Immunoassays
- Nur Binte: Evaluation of Coatings for Protein Immobilization on Polymer Surfaces
- Joel Britschgi: Development of a Regenerable Microarray-based Receptor Assay for the Detection of Tetracyclines
- Julia Neumair: Isothermal Amplification and Live/dead Differentiation of living Legionella in Real Sample on the MCR 3
- Leonhard Prechtl: Development of a Direct-Competitive Microspot Upconversion-Linked Immunosorbant Assay (MULISA) for Diclofenac in Microtiter Plate Format
- Cindy San: A Fast Concentration Method for *Escherichia Coli* Based on Monolithic Immunoaffinity Extraction

Christian Schröder: Quartz-enhanced Photoacoustic Spectroscopy of NO<sub>2</sub> and Soot Li Yan Tay: Evaluation of Turbidity Influences on Monolithic Adsorption Filtration Markus Weber: Investigations into On-line Determination of Soot Reactivity Marlene Weyerer: Application of Bacteria as Non-Specific Toxicity Probes

## Institute Colloquia

- Prof. Dr. Andrew Ewing, University of Gothenburg, Department of Chemistry & Molecular Biology: Electrochemistry and Mass Spectrometry Imaging in Flies, Cells, and Vesicles (9.5.2016)
- Prof. Dr. Michael Wagner, Head of Department of Microbiology and Ecosystem Science, Division of Microbial Ecology, University of Vienna: Tracking the Activity of Microbes in the Environment and in Hosts Using Raman Microspectroscopy- and NanoSIMS-based Single Cell Isotope Probing Techniques (23.5.2016)

- Dr. Werner Lehmann, Attomol GmbH, Molekulare Diagnostika, Bronkow: Multiplex Bead Assays: A Novel Technology for Medical Routine Diagnostics (21.9.2016)
- Prof. Dr. Zeyad Alwahabi, School of Chemical Engineering, University of Adelaide, Australia: Laser Diagnostics: From Science to Application (4.10.2016)
- Prof. Dr. Sonja Berensmeier, Technische Universität München, Department of Mechanical Engineering, Bioseparation Engineering Group: Bioseparation Engineering – Interface between Life Sciences and Engineering (6.10.2016)
- Prof. Dr. Stefan Dübel, TU Braunschweig, Institute of Biochemistry, Biotechnology and Bioinformatics: In Vitro Evolution for the Generation of Designer Antibodies (14.11.2016)

## **External Tasks and Memberships**

## T. Baumann

<ul> <li>Baumann</li> <li>Bayer. Fachausschuss für Kurorte, Erholungsorte &amp; Heilbrunner</li> <li>VBEW Arbeitskreis Wasserschutzgebiete</li> <li>Arbeitskreis Spurenstoffe im Umweltcluster Bayern</li> <li>Network Innovative Landfill Techniques (iDetec)</li> </ul>	n Deputy Member Guest Member Member Member
C. Haisch Kommission Reinhaltung der Luft im VDI und DIN - Normen- ausschuss: Unterausschuss Messen von Partikeln in der Außenluft - Bestimmung der Partikelanzahl	Member
D. Knopp Chromatographia Ecotoxicology and Environmental Safety International Journal of Environmental Research and Public Health	Editorial Advisory Board Editorial Advisory Board Editorial Advisory Board
School of Chemical Engineering, National Technical University of Athens (NTUA), Greece. Election committee	Member
R. Niessner Bayer. Fachausschuss für Kurorte, Erholungsorte & Heilbrunner Heinrich-Emanuel-Merck Award fms_ProcesNet-Gemeinschaftsausschuss Sensoren und Sensorsysteme (DECHEMA)	n Member Jury Head Member
Analytical Chemistry Analytical & Bioanalytical Chemistry Analytical Sciences Fresenius' Environmental Bulletin International Journal of Environmental Analytical Chemistry Microchimica Acta	Associated Editor Advisory Board Member Advisory Board Member Advisory Board Member Advisory Board Member Advisory Board Member

	visory Board Member
Toxicological & Environmental Chemistry Adv	visory Board Member
M. Seidel	
ausschuss: Unterausschuss Messen und Bewerten von Legio-	ember
nellen	
Kommission Reinhaltung der Luft im VDI und DIN - Normen- Me ausschuss: Arbeitsgruppe "Bioaerosole und biologische Agenzien – Luftgetragene Mikroorganismen und Viren"	ember
Spiegelgremium zur CEN/TC 264/WG 28 "Microorganisms in Me ambient air"	ember
Fachgruppe für "Viren und Parasiten" bei der Wasserche- Me mischen Gesellschaft in der GDCh	ember

# Teaching

## **GIST TUM-Asia**

## Industrial Chemistry (M.Sc.)

Bioengineering & Bioprocessing; Seidel Hydrochemistry; Niessner

## **Chemical Engineering (B.Sc.)**

Biochemical Process Engineering; Seidel

## Biosciences (B.Sc./M.Sc.)

Analytical Chemistry - Separation Techniques, Chemical and Biochemical Sensors (Analytische Chemie -Trenntechniken, chemische und biochemische Sensoren); Knopp **Biochemical and Molecular Biological** Methods in Environmental Analysis I -Immunological methods; Sensor techniques (Biochemische und molekularbiologische Verfahren ind er Umweltanalytik I - Immunologische Methoden, Sensor Techniken); Knopp **Biochemical and Molecular Biological** Methods in Environmental Analysis II -Enzymatic methods; DNA Probes (Biochemische und molekularbiologische Verfahren in der Umweltanalytik II -Enzymatische Methoden, DNA-Sonden); Knopp

# Chemistry (B.Sc./M.Sc.)

Hydrogeological, Hydrochemical and Environmental Analysis Seminar (Hydrogeologisches, Hydrochemisches und Umweltanalytisches Seminar); Niessner, Baumann, Haisch, Knopp

Graduate Course in Analytical Chemistry: Lecture in Organic Trace Analysis-Physical and Chemical Separation Methods (Nebenfach Analytische Chemie:Vorlesung Organische Spurenanalytik-Physikalisch-chemische Trennmethoden); Niessner

Graduate Course in Analytical Chemistry: Lecture in Organic Trace Analysis-Applications of Selective Receptors (Nebenfach Analytische Chemie: Vorlesung Organische Spurenanalytik-Nutzung selektiver Rezeptoren); Niessner, Seidel

Graduate Course in Analytical Chemistry: Lab in Organic Trace Analysis (Nebenfach Analytische Chemie: Kurspraktikum Organische Spurenanalytik); Niessner, Seidel

Graduate Course in Analytical Chemistry: Research Lab in Organic Trace Analysis (Nebenfach Analytische Chemie: Forschungspraktikum Organische Spurenanalytik); Niessner, Seidel

Trace Analysis Techniques (Spurenanalytische Techniken); Niessner, Knopp, Haisch

# Geosciences (B.Sc./M.Sc.)

Analytical Chemistry I: Instrumental Analysis for Geoscientists (Analytische Chemie I: Instrumentelle Analytik für Geowissenschaftler); Niessner Analytical Chemistry II - Organic Trace

Analysis for Geoscientists (Chemische Analytik II - Organische Spurenanalytik für Geowissenschaftler); Niessner

Contaminant Hydrogeology (Transport von Schadstoffen im Grundwasser); Baumann

Remediation Design (Erkundung und Sanierung von Grundwasserschadensfällen); Baumann

Technical Hydrogeology (Technische Hydrogeologie); Baumann

Fluidflow in Porous Media Lab (Hydrogeologisches Laborpraktikum); Baumann, Haisch, Niessner

Hydrogeochemical Modelling (Hydrogeologische Modellierung II); Baumann

Hydrogeological Field Lab (Hydrogeologische Feldmethoden); Baumann

Hydrogeological Mapping (Hydrogeologische Kartierung); Baumann

Hydrogeological and Hydrochemical Field Trips (Hydrogeologische und Hydrochemische Exkursion); Baumann

Water Chemistry I (Wasserchemie I); Niessner Water Chemistry II - Hydrocolloids, Micellar Systems and Photochemical Transformations (Wasserchemie II -Hydrokolloide, micellare Systeme und photochemische Umsetzung); Niessner Hydrochemical Lab (Hydrochemisches

Praktikum); Knopp, Baumann

# Equipment

### 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

Großhadern Unsaturated Zone field laboratory (10 m deep)

1 Analytical Autoclave, Büchi Midiclave

#### **Dioxin Laboratory**

3 High security labs with locks, separate activated carbon filter and highperformance particle filter systems

#### Aerosol Research

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

#### Bioseparation

- 1 Crossflow-ultrafiltration unit (6 m<sup>2</sup>-hollow fibre module, Inge-AG)
- 1 Munich Microorganism Concentrator (MMC 3)
- 1 Monolithic Affinity Filtration Unit

#### Molecular Biology

- 1 Biacore X100, General Electric
- 1 Real-time PCR (Light Cycler 480, Roche)

#### Microarray Technology

- 2 Chemiluminescence Microarray Reader (Immunomat, IWC)
- 4 Chemiluminescence Microarray Reader (MCR 3, GWK GmbH)
- 1 Ink-Jet Microdispenser (SciFlexarrayer 31, scienion)
- 2 Contact Microarrayer (BioOdyssee Caligrapher, BioRad)
- 1 Cutting Plotter (Graphtec CE6000-40)

#### Microbiology

- 1 Flow Cytometer (Cell Lab Quanta SC, Beckman Coulter)
- 1 Flow Cytometer (CyFlow Cube 6, Sysmex Partec GmbH)
- 1 Water Microbiology (Colilert-18 and Quanti-Tray 2000, IDEXX)
- 3 Clean benches
- 1 Microbiological Incubator (BD 53, Binder)
- 1 Autoclave (Century 2100, Prestige Medical)
- 1 Autoclave (SHP Steriltechnik)
- 1 Bio-2-Aerosol Chamber

#### Standard Lab Equipment

- 1 Lyophilizer (Alpha 1-4 LSC, Christ)
- 1 Washer Disinfector (DS 500 Lab, International Steel CO.SPA)
- 1 Ultrapure Water System (Direct-Q 3 UV, Millipore)
- 1 Refrigerated Centrifuge (Universal 320R, Hettich)
- 1 Centrifuge (Eppendorf 5804 R)
- 1 Climatic chamber (Memmert HCP 108)
- 2 Fluorescence reader systems, timeresolving
- 3 Photometric reader systems
- 1 384-channel washer, Biotek
- 1 Turbidometer (WTW GmbH)
- 1 Nanophotometer (Implen GmbH)

### Chromatography and Particle Separation

- 3 GCs with FID, NPD, ECD, TEA, and AED
- 1 Orbitrap-based benchtop MS, Exactive/ HCD-System, Thermo Fischer
- 1 GC/MS, VG Autospec
- 1 GC/MS, Shimadzu
- 1 Portable Micro-GC, MITEC
- 1 Asymmetrical Field-flow-fractionation system, Postnova
- 2 Concentrators for dynamic headspace analysis
- 4 HPLC, UV/VIS array detector, programmable fluorescence detector
- 1 Capillary electrophoresis system
- 1 Ion chromatograph, Dionex 4500 i
- 1 Ion chromatograph, Dionex BioLC (Photodiode Array Detector, Electrochemical Detector)
- 1 Ion chromatograph, Metrohm 881
- 1 LC system, ECONO
- 1 Preparative HPLC
- 1 Zetaphoremeter, SEPHY

### **Elemental Analysis**

- 1 TXRF, Atomika EXTRA II a
- 1 Flame-Photometer, Eppendorf ELEX 6361
- 2 AAS systems with flame atomization, electrothermal atomization, hydrid system, Perkin-Elmer PE 3300, ELAN 4100
- 1 ICP-MS, Perkin-Elmer Nexion 350D

## Laser

- 2 He/Ne-laser
- 5 Nd-YAG-laser, pulsed
- 1 Nd-YAG Laser 2 W cw, 532 nm narrow band
- 3 Nd-YAG-laser, cw
- 1 CO<sub>2</sub>-laser
- 3 Dye-laser (tunable with frequency doubler)
- 5 N<sub>2</sub>-laser
- 8 Diode-lasers (600-1670 nm; up to 2 W CW)
- 1 Laserdiode array with 10 diodes (0.8 μm -1.8 μm)
- 1 Laserdiode with external resonator
- 2 Optical parameter oscillator (410 nm 2.1 µm)

## Optoelectronics/Spectrometer

- 1 Rowland spectrometer
- 2 Echelle spectrometer
- 1 ICCD spectrometer system
- 1 FTIR-Spectrometer, Thermo Scientific Nicolet 6700
- 1 Fluorescence spectrometer, Perkin Elmer LS-50
- 1 Fluorescence spectrometer, Shimadzu RF 540
- 1 Fluorescence spectrometer, Shimadzu RF 5301 PC
- 1 UV/VIS spectrometer, Beckman DU 650
- 1 UV/VIS spectrometer, analytic jena Specord 250 plus
- 1 UV/VIS spectrometer, analytik jena Spekol 1500
- 2 Boxcar integrator
- 4 Digital storage oscilloscopes (400 MHz, 500 MHz)
- 3 Optical multichannel analysators with monochromators, time-resolving
- 1 Wavemeter

## SEM/Microscopy

- 1 SEM/EDX system, Zeiss Gemini
- 1 Polarisation microscope for phase analysis
- 1 Fluorescence microscope
- 1 Image analysis software for automated image processing
- 1 Inert gas glovebox
- 1 Laminar flow box

## Raman-Microscopy

- 1 Laser Raman microscope, WITec alpha300R (532/633 nm)
- 1 Laser Raman microscope, Renishaw 2000 (514/633/785 nm)
- 1 Laser Raman microscope, Horiba LabRam HR (532/633/785 nm)
- 1 Temperature controlled stage (-196°C 600°C, Linkam THMS 600)

## Sum Parameters

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

## **Staff 2016**

#### Staff

Univ.-Prof. Dr. Reinhard Niessner PD Dr. Thomas Baumann PD Dr. Christoph Haisch Dr. Natalia Ivleva Prof. Dr. Dietmar Knopp PD Dr. Michael Seidel

#### **Birgit Apel**

Christine Beese Roland Hoppe Mira Kolar Joachim Langer Susanne Mahler Cornelia Popp Hatice Poyraz Christine Sternkopf Sebastian Wiesemann

#### PhD Students

MSc Pharm. Biol. Manuela Adebar MSc Wasserb. Sayed Amininejad MSc Chem. Philipp Anger (9/16-) MSc Chem. David Bauer (12/16-) MSc Chem.-Ing. Jonad Bemetz Exam. Lebensm. Chem. Carolin Hartmann (1/16-) MSc Chem. Stefan Heberle Dipl.-Biol.-Ing. Dennis Elsäßer (-7/16) MSc Chem. Michaela Eß (-9/16) MSc Chem. Bettina Kiwull (-5/16) MSc Chem. Catharina Kober MSc Erdw. Bernhard Köhl MSc Chem. Patrick Kubryk MSc Chem. Andreas Kunze (-1/16) MSc Chem. Verena Meyer MSc Chem. Anna-Cathrine Neumann (-5/16) MSc Pharm. Angelika Nistler MSc Chem. Li Qiu (10/16-) MSc Chem. Alexander Rinkenburger MSc Bio. Chem. Sandra Schäfer MSc MBT Katharina Stutzer MSc Chem. Klemens Thaler MSc Geol. Martina Ueckert MSc Chem. Ruben Weiß (2/16-) MSc Chem. Alexandra Wiesheu MSc Chem. Carina Wismeth Exam. Leb. Chem. Anika Wunderlich (-4/16)

## External PhD Students

MSc Chem. Michael Göttel MSc Toxikologie Anne Landmesser (3/16-) MSc Biochem. Stefanie Mak (1/16-) MSc Biol. Johannes Otto (-2/16) Dipl.-Biol. Michael Schmalenberg MSc Biochem. Ruoyu Sun

#### Diploma Students / Master Students

BSc Chem. Philipp Anger (3/16-8/16) BSc Chem Nadine Berger (-2/16) BSc Leb. Chem. Sebastian Dirndorfer (-6/16) BSc Chem.-Ing. Fabian Hagen (10/16-) BSc Chem. Ryan Karongo (6/16-12/16) BSc UPIÖ Constanze Neumann (11/16-) BSc Chem. Veronika Stiegler (1/16-7/16)

#### Bachelor Students

Christian Biermaier (4/16-6/16) Nur Binte (-2/16) Joel Britschgi (4/16-7/16) Julia Neumair (5/16-7/16) Leonhard Prechtl (8/16-10/16) Cindy San (-2/16) Christian Schröder (4/16-7/16) Mei Xi Tan (12/16-) Li Yan Tay (-2/16) Markus Weber (3/16-5/16) Marlene Weyerer (4/16-6/16)

## **Guests and Research Fellows**

Dr. Nicoleta Dina (5/16-6/16) Adomas Griauslys MSc (-1/16) James Grundy (5/16-7/16) Dr. Anna Cathrine Neumann (8/16-) Dr. Genny Pang Laura Sanchez (3/16-8/16) Aleksandr Sobelev PhD (10/16-) Bastian Striebel (5/16-) Meng-Che Tu (-3/16) Dr. Jan-Christoph Wolf (5/16-) Dr. Klaus Wutz (4/16-)

#### Student Assistants

Steffen Amann (-1/16) Philipp Anger (-8/16) Jessica Beyerl Bastian Striebel (-4/16)