HelmholtzZentrum münchen
Deutsches Forschungszentrum für Gesundheit und Umwelt

HICE

Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health

www.hice-vi.eu

HICE › Aerosols and Health
Helmholtz Virtual Institute of Complex
Molecular Systems in Environmental Health

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Ralf Zimmermann HICE Spokesperson Head of the JMSC

Dear Reader,

The term "environmental health", as it is defined by the World Health Organization, comprehends those aspects of human health and disease that are determined by factors in the environment. It also refers to the theory and practice of assessing and controlling those factors in the environment that can potentially affect health. “Environment” is a general term in this context and may additionally comprehend two classical environmental factors, air and water pollution, including, for example, life-style and psychological factors.

In the developed world air pollution represents one particularly important classical factor for environmental health. Numerous epidemiological and toxicological studies have proven that human health and well-being are substantially impacted by anthropogenic air pollution. In the urban aerosol, the mixture of airborne particulate matter and reactive gases is of relevance for the observed acute and chronic health effects. A recent report of the World Health Organization, WHO, concluded that man-made particulate emissions from combustion sources together with its content of transition metals and organic compounds are particularly important for human health effects. This existing knowledge thus renders the anthropogenic urban aerosol one of the major topics of environmental health research.

In the context of this background, I’m very delighted to be able to disclose that the “Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health” (HICE) with the focus topic “Aerosols and Health” was launched on January 1, 2012. The official inauguration of this large research project network will take place on May 8, 2012, at the Leibniz Institute for Baltic Sea Research in Warnemünde. The

scientific ideas of this research initiative were partly elaborated during a workshop I organised at the Analytica Conference and at the Helmholtz Zentrum München in 2010. The HICE topics and network were developed and proposed to the Helmholtz Association (HGF) by the Joint Mass Spectrometry Centre of the Helmholtz Zentrum München and the University of Rostock (JMSC). After a competitive review and assessment process, HICE was finally approved and will now be funded by the HGF for five years with a total of five million Euros.

HICE consists of work groups from eight partner institutions: the Helmholtz Zentrum München (HMGU), the Max Delbrück Center (MDC), the Karlsruhe Institute of Technology (KIT), the University of Rostock (UR), the Technische Universität München (TUM), the University of Eastern Finland (UEF), the University of Cardiff (UCA), the University of Luxembourg (ULU) and a number of associated partners.

In the subsequent years, HICE will particularly address aerosol-related health effect mechanisms, the health importance of organic compounds in anthropogenic aerosol, potential synergistic effects of reactive gas-phase compounds and particles for inducing health effects and the influence of the increase in biomass burning and biofuel use on aerosol composition and related health effects. To accomplish these research tasks, innovative analytical, bio-analytical and toxicological methods will be applied. This includes novel and highly innovative on-line and off-line aerosol analysis technologies, and new lung-cell based concepts for toxicological and biochemical effects assessment.

Last but not least, it must be stated that a clear aim of the HICE activity is structure and capacity building for both the research consortium and for the Joint Mass Spetrometry Centre (JMSC) core cooperation between the University of Rostock and the Helmholtz Zentrum München.

I look forward to an exciting research program and interesting scientific results in the field of environmental health with the focus on anthropogenic aerosols.

Rostock, March 24, 2012

Prof. Dr. Ralf Zimmermann

Spokesperson of HICE
Head of the Joint Mass Spectrometry Centre (JMSC)
of the University of Rostock and the Helmholtz Zentrum München

Aim, Strategic Partnership and Structure

THE "HELMHOLTZ VIRTUAL INSTITUTE OF COMPLEX MOLECULAR SYSTEMS IN ENVIRONMENTAL HEALTH" (HICE) WAS FOUNDED ON JANUARY 1, 2012.

Aim

HICE is represented by the spokesperson Prof. Dr. Ralf Zimmermann (Joint Mass Spectrometry Centre of the Helmholtz Zentrum München and the University of Rostock) and comprehends funded work groups from eight partner institutions.

HICE Partner Institutions

Helmholtz Zentrum München (HMGU)
Max Delbrück Center Berlin-Buch (MDC)
Karlsruhe Institute of Technology (KIT)
University of Rostock (UR)
Technische Universität München (TUM)
University of Eastern Finland (UEF)
University of Cardiff (UCA)
University of Luxembourg (ULU)

Furthermore, five associated partners have joined the network.

The objective of the HICE is the establishment of a long-term scientific research initiative for the investigation of the causes and mechanisms of environmentally influenced diseases. In the initial phase, HICE will focus on a deeper understanding of the impact of anthropogenic aerosols on human health. Based on current hypotheses, reactive organic compounds in particle as well as in gas phase of aerosols are particularly relevant.

Innovative in-vitro human lung tissue models are exposed to aerosols and separated gas and particle phases from relevant sources.

The response of the biological systems is investigated by state-of-the art analytical techniques on different biological levels (transcriptome, proteome, metabolome, toxicological parameters). A unique approach is the application of novel mass spectrometry-based analytical methods for comprehensive, non-targeted analyses of small molecules in combination with stable isotope labelling approaches for detection of flux changes in the metabolism. The complex biological response data is chemometrically and bio-statistically analysed in conjunction with comprehensive chemical and physical data of the aerosol used for exposure in order to identify biomarkers of exposure, harm and disease.

In general, a Helmholtz Virtual Institute brings together the key competencies of one or more Helmholtz Centres with those of one or more universities to create a centre of excellence of international standing. The Helmholtz Virtual Institutes are co-funded by the Initiative and Networking Fund (INF) of the Helmholtz Association (HGF). Helmholtz Virtual Institutes shall establish and extend research partnerships between Helmholtz Centres and German universities, generate new collaborations with leading international partner institutions and provide a distinct

benefit in preparing the way for larger strategic research projects such as the Helmholtz Alliances and Institutes. With the funding mechanism the Helmholtz Association wants to strengthen the position of universities in the German scientific system.

Strategic Partnership

The Joint Mass Spectrometry Centre (JMSC) of the Helmholtz Zentrum München (HMGU, Cooperation Group "Comprehensive Molecular Analytics") and the University of Rostock (UR, Chair of Analytical Chemistry) form the inner circle of HICE. The analytical and aerosol-physical expertise of the JMSC is complemented by biological, engineering and clinical-toxicological expertise of further institutes of the Helmholtz Zentrum München and the University of Rostock and the Technische Universität München (TUM), the Karlsruhe Institute of Technology (KIT) and the Max Delbrück Center (MDC). Three outstanding international partners, the University of Luxembourg (ULUX), the University of Cardiff (UCA) and the University of Eastern Finland (UEF) as well as associated partners from commercial business and non-university research institutions complete the expertise profile of HICE.

Structure

In addition to bringing together complementary techniques, the Virtual Institute implements new organisational structures to ensure the success of different interdisciplinary groups to one interacting institute and to build a long-term structure. This enables the consortium to attract sufficient third-party funds to accomplish the research tasks.

The interdisciplinary research of HICE is structured in four well-defined interrelated work packages. In addition, HICE includes a management structure supervised by a joint scientific steering board.

Education

HICE is also devoted to the education of graduate students and the promotion of young scientists by means of a joint graduate school program and by establishing a young investigator group. Using internet-based seminars and video transmitted lecture series, the expertise of all national and international partners is available.

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Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health HICE

Virtual Institute Scientific Steering Board (VISB)

Spokesperson HICE: Prof. Dr. Ralf Zimmermann (HMGU, UR)
Spokespersons Work Packages: Prof. Jorma Jokiniemi (UEF), Dr. Hanns-Rudolf Paur (KIT), Dr. Gunnar Dittmar (MDC), N.N.

Virtual Institute Management and Administration (VIMA)

Project Management: Sorana Scholtes

Work Package I
Aerosol Characterisation

WP Spokespersons:

1. Prof. Jorma Jokiniemi (UEF)

2. Dr. Thorsten Streibel (UR)

Work Package II
Exposure and Toxicology

WP Spokespersons:

1. Dr. Hanns-Rudolf Paur (KIT)

2. Prof. Dr. Jeroen Buters (TUM)

Work Package III
Small Molecules and Stable Isotope Labelling

WP Spokespersons:

1. Dr. Gunnar Dittmar (MDC)

2. Thomas Gröger (HMGU)

Work Package IV
Chemometry and Biostatistics

WP Spokespersons:

1. N.N.

2. Prof. Dr. Olaf Wolkenhauer (UR)

Scientific Background and Motivation

THE SEVERE IMPACT OF AIR POLLUTION ON HUMAN HEALTH IS A WELL-ESTABLISHED PHENOMENON SINCE THE INDUSTRIAL REVOLUTION.

Aerosols by definition are solid or liquid particles suspended in a gas phase. In epidemiological studies on health effects of ambient particulate matter (PM) the mass concentration of particulate matter in ambient air is often correlated with observed health effects. Many studies investigated the effects of PM2.5 mass (particles with an aerodynamic diameter smaller than 2.5 µm) on morbidity and mortality. In figure 2, the estimated averaged loss of life expectancy (LLE) per inhabitant due to PM–related health effects in Europe is given as a colour coded map. In central Europe the estimated LLE exceeds 6 months in most places. In regions with high PM concentration, such as the Po Valley in Italy or the densely populated areas in North Rhine-Westphalia (Germany), the Netherlands and Belgium, there was a 12 months LLE exceedance. This renders the research field "health effects of aerosols" an extremely important topic in environmental health research.

While the total mass of PM2.5 has been associated with adverse human health outcomes, the relationship between these and specific particle characteristics (e.g. surface area) or chemical components has not yet been resolved. Furthermore, there is a growing concern that high emissions of oxygenated compounds from novel fuels such as biodiesel [3] increase the toxicity of emissions from respective sources. Recently, also cytotoxicity and genotoxicity of volatile organic compounds from wood combustion were investigated in human lung cells [4].

Cell line applications are easier to control, cheaper to set up and better to interpret than adaptations of whole animal models and human beings [5]. Metabolomic analysis of human cell models in conjunction with other comprehensive analyses at different hierarchical levels (e.g. proteomics and transcriptomics) provides information on the system level and helps in the verification of unknown biological pathways [6, 7]. Although during the last years scientific efforts to identify mechanisms of health impairments caused by aerosols increased dramatically, the most urgent questions remain unacknowledged.

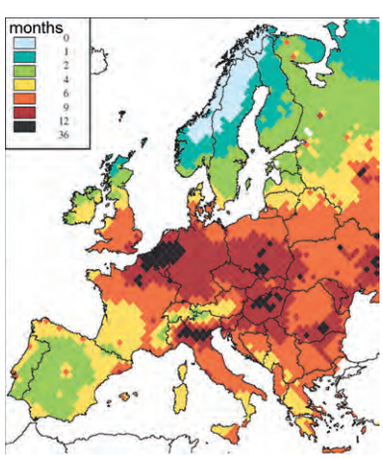


Fig. 2: Loss of life expectancy (months) attributable to exposure to fine particulate matter (PM2.5) in 2000; source: EU-Clean Air Force Europe (CAFE).

Scientific Hypotheses and Approach

THE GENERAL CONCEPT CAN BE SUMMARISED AS CONTROLLED EXPOSURE OF BIOLOGICAL MODEL SYSTEMS WITH FRESH (I.E. REACTIVE) AEROSOLS FROM RELEVANT ANTHROPOGENIC SOURCES ACCOMPANIED BY STUDIES OF THE BIOLOGICAL EFFECTS ON THE DIFFERENT BIOLOGICAL HIERARCHIES.

The combination of comprehensive chemical analysis of small molecules with toxicological, transcriptome, proteome and metabolome analysis by chemometrics and biostatistics permits the revelation of biomarkers.These markers are subsequently used for ethically sound clinical studies. As a longterm goal the developed and established strategy for biomarker recognition shall be applicable for similar scientific questions.

HICE combines national and international expertise in analytical chemistry, aerosol science and chemical toxicology within a new concept. This concept is driven by three scientific hypotheses.

Scientific Hypotheses

1) Reactive organic compounds in ambient aerosols present either in the gas phase or the particle phase or in both phases are particularly relevant for the induction of the observed adverse health effects.

2) Synergistic effects of reactive organic compounds in the gas phase and the particulate phase play an important role in causing these effects.

3) The expected strong increase in the use of biomass and biofuels will change the composition and properties of the (urban) aerosol and may lead to more or other health effect implications. The scientific work of HICE shall either support or disprove these hypotheses. The concept (see 3) can be described by the following essential topics:

- Comprehensive chemical and physical characterisation of the aerosol, using state-of-the art on-line and off-line techniques such as aerosol mass spectrometry (AMS/ATOF), comprehensive multidimensional chromatographic and high resolution mass spectrometric technologies for particle analysis or photo ionisation mass spectrometry for the identification and determination of reactive gas-phase compounds.

- Use of controlled, partially mobile exposure technology which allows the differentiated exposure of biological systems with either the freshly emitted whole aerosol, e.g. from engines or solely the reactive gas or particle phase in order to differentiate particle and gas phase induced health effects and elucidate synergistic effects.

- Application of newly established differentiated human lung cell cultures simulating the surface of the human lung for controlled exposure experiments at the air-liquid interface (ALI).

- Thorough and comprehensive state-of-the-art characterisation of the biological effects of the transcriptome, proteome and metabolome including toxicological tests and phenotypical description, partially by using innovative mass spectrometric (MS) technologies, such as ultra-high resolution MS (Fourier transform ion cyclotron resonance mass spectrometry, FTMS) or isotope-ratio analyses (IRMS).

- Combination of both innovative comprehensive chemical analysis methods for small molecules based on multidimensional chromatographic and mass spectrometric technologies as well as isotope labelling methods allows profound and sensitive investigation of metabolic fluxes and changes in the proteome. This approach promises a high sensitivity to detect early onsets of adverse effects.

- Joint analysis of exposure and biological response data by chemometrical and biostatistical approaches to identify health relevant fractions and substances as well as stable and significant biomarkers for the initial steps of disease formation.

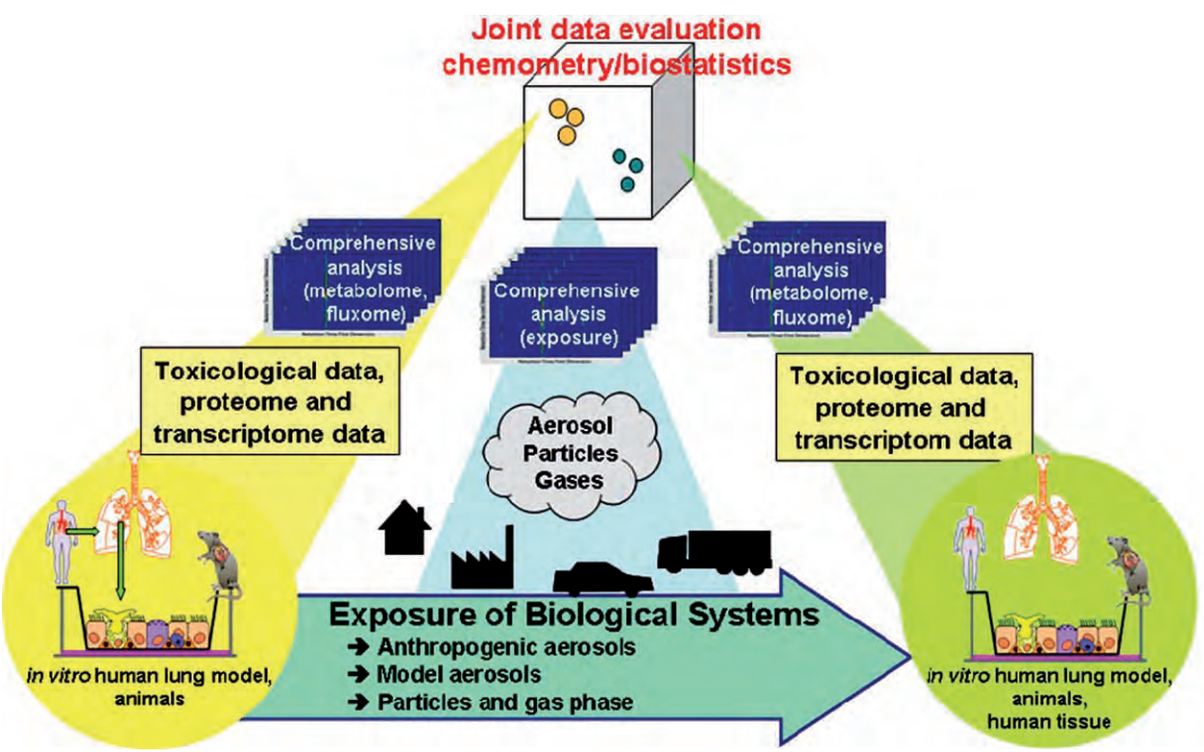
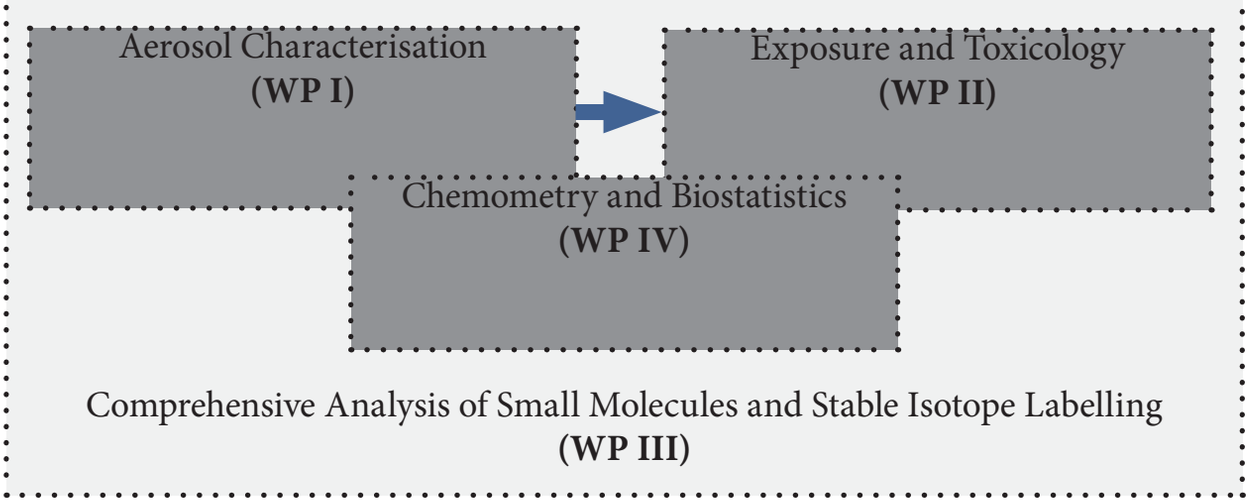


Fig. 3: HICE scientific approach: In-vitro human lung model is exposed in a defined character to fresh anthropogenic combustion aerosols. The biological repose is comprehensively characterised. Joint bioinformatical data analysis is aims at the detection of biomarkers.

HICE Work Packages



Work Package I

IN WP I THE AEROSOLS FROM A LARGE VARIETY OF ANTHROPOGENIC SOURCES AND MODEL AEROSOLS ARE CHARACTERISED WITH RESPECT TO REACTIVE ORGANIC COMPOUNDS AND PROVIDED FOR EXPOSURE EXPERIMENTS.

Characterisation of Reactive Organic Compounds in Gases and Particulate Matter

Emissions of typical anthropogenic combustion sources are investigated. The consortium has a wide range of technical equipment at the University of Western Finland and at the University of Rostock: boiler burners, automotive engine test setups and marine diesel engines. For tests and standard reference measurements flame soot and ash particles are prepared. Modern fuel formulations (biofuel) that are known to hold a higher oxygen content are taken into account.

Modern methods of mass spectrometry and measurement techniques for chemical and physical methods are applied to characterise the emission aerosol comprehensively. Both resonance enhanced multi photon ionisation and single photon ionisation set up the basis for the mass spectrometric methods.

The reactive organic compounds (ROC) in the gas phase of the aerosol are characterised by photoionisation – mass spectrometry, the particles by aerosol – time-of-flight-mass-spectrometry (ATOF). Additionally, physical parameters of the particles, like number and mass concentration are determined on-line.

During work in progress, the analytical focus will be shifted to the potential recurrent markers which are based on the results determined in WP II and WP III. The aim is an emission assessment based on (bio-) statistical concepts which combine the results of WP I with those of the analytical approaches in WP II and WP III.

In 2012, test campaigns for realigning analytical methods as well as tests of newly built up air-liquid-interface exposure units will be carried out at a wood combustion facility in Germany and at the Chair of Piston Machines and Internal Combustion Engines in Rostock. The first intensive measurement campaign will be carried out in February and March 2013 at the Vehicle Emissions Laboratory (VELA) of the Joint Research Centre in Ispra, Italy. In this campaign, emissions from vehicles using different biofuel mixtures under cold start and driving conditions are the focus of the investigation.

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Work Package II

IN WP II THE BIOLOGICAL EFFECTS OF THE FRESHLY GENERATED COMBUSTION AEROSOL, THE PARTICLE PHASE ALONE AND THE GAS PHASE ALONE ARE STUDIED COMPARATIVELY IN HUMAN CELLS.

Health Effects and Toxicology of Reactive Organic Compounds in Aerosols

The cells are exposed to the aerosol both in vitro and in an exposure equipment at the air-liquid-interface (ALI). In co-cultures up to five cell types are combined with a differentiated human lung tissue model. By in-vivo studies the results are transferred to human specimen. The biological effects in cell cultures and tissues are investigated on all hierarchical levels (transcriptome, proteome and metabolome).

The biological effects are examined together with WP III. The biological endpoints therefore are, e.g., cytotoxicity, metabolic activity, determination of functions, oxidative stress and inflammatory response markers. In addition, non-targeted effects are addressed by the basis of genome-wide gene expression, protein profiles and induction analyses. In selected experiments, stable isotope labeling is used to perform flux analyses in proteome and metabolome.

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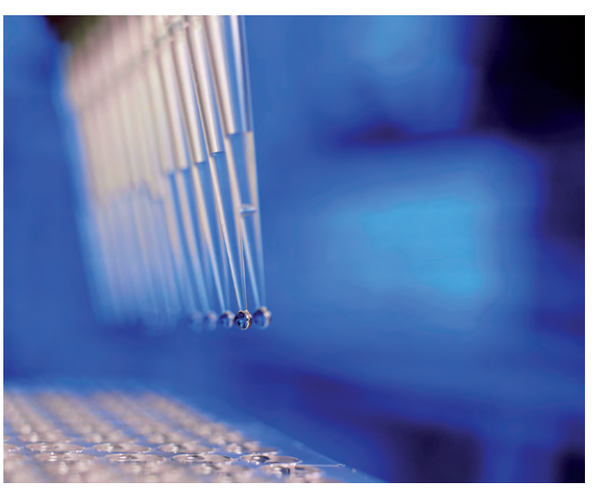

Image source: Helmholtz Zentrum München.

Work Package III

THIS WORK PACKAGE HAS ITS FOCUS ON COMPREHENSIVE CHEMICAL ANALYSIS.

Comprehensive Chemical Analysis of Small Molecules in Aerosols and Biological Systems

This is the investigation of the impact of chemically and physically well-characterised aerosols on biological test systems and their potential health effects. Therefore, the changes in the pattern of small molecules in biological test systems caused by the impact of aerosols will be investigated.

A broad spectrum of mass spectrometric and chromatographic techniques is established (LC, GC, TOFMS, FTMS, MALDI imaging). Much research work has been done to facilitate the quantitative analysis of large time series and the analysis of selected marker compounds. Concepts for a comprehensive chemical profiling (GCxGC) and isotopic labelling "non-targeted tracer fate detection (NTFD)" have been established and applied to environmental and/or biological applications.

The NTFD concept is applied to cell cultures to investigate the effects of aerosols on biological systems. In a second step the NTFD methodology is combined with comprehensive two-dimensional gas chromatography (GCxGC).

Therefore, targeted and non-targeted methodologies are applied. FTMS and IRMS systems are used for marker identification and chemical profiling of aerosols and biological systems.

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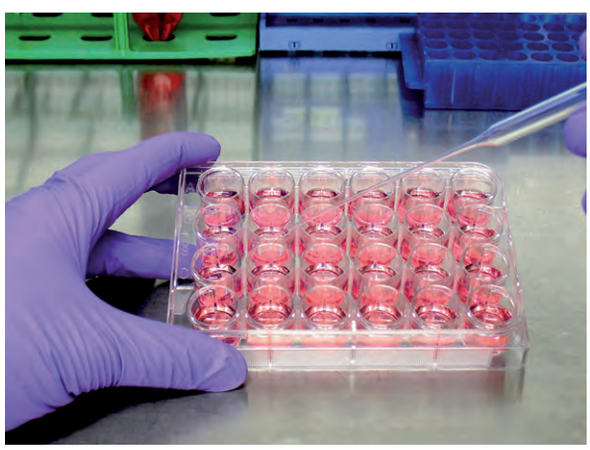

Image source: Vitrocell.

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Work Package IV

WP IV IS A CENTRAL INTERFACE WITHIN THE FRAMEWORK OF HICE. IT IS RESPONSIBLE FOR THE COMBINED STATISTICAL DATA ANALYSIS COMPRISING ALL ANALYTICAL WORK PACKAGES (WP I-III).

Scientific Data Management, Chemometrics and Biostatistics

First, it needs to be set up and the data management of all scientific data must be supervised. Beside this standing facility, WP IV supports the different projects within the WPs with the "design of experiment (DOE)" to guarantee the applicability of statistical methods and documentation of the experiment. A third task is the central analysis and evaluation of scientific data and a basic consistency check. For a comprehensive analysis of the data, results from the WPs are linked and joined together within and between the WPs for a biostatistical analysis.

WP IV assists the scientists of the WP I-III with DOE and concepts for data handling and processing. WP IV performs the common statistical analysis to link data between different analytical platforms, concepts or WPs. Data from all measurement campaigns and exposure experiments are statistically evaluated and comprehensively interpreted with respect to potential biomarkers for health effects caused by aerosols.

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Image source: Helmholtz Zentrum München

Education

ONE OF THE MAIN TASKS OF HICE IS THE PROMOTION OF STUDENTS, PHD STUDENTS AND YOUNG RESEARCHERS.

The Helmholtz Virtual Institute unites a diversity of scientific disciplines including chemistry, physics, medicine, biology and bioinformatics from different national and international institutions. Thus it provides an excellent frame for graduate student education which will be fulfilled implementing a joint interdisciplinary Graduate School (GS) for Complex Molecular Systems in Environmental Health.

Offers of the Graduate School

Lectures and Seminars
A joint scientific seminar series is conducted weekly during the academic term where progress reports from HICE activities are given. In addition a lecture series is organised where internal and external experts give overview lessons on science and technological topics. These activities are transmitted via video conference to all partner institutions.

Interlaboratory Exchange
The partnering institutions organise an exchange of young scientists and technical staff between different laboratories of the partner institutes.

Regular Workshops
Periodic meetings are organised, where scientific staff of all involved institutions is present. On this scientific platform, young scientists are educated and trained to present scientific results.

Summer Schools
HICE annually organises summer schools at partner institutions. Depending on the expertise of the respective host institution, different key issues are covered. The courses consist of practical work as well as expert lectures and thus contribute to the professional development of the attendants.

Mentoring
PhD students are supported by thesis committees, comprising two mentors chosen by the student and the doctoral thesis supervisor, respectively. Post-docs are accompanied by a mentor for scientific career advising.

Image source: Helmholtz Zentrum München

Outlook and Long Term Strategy

HICE INTENDS TO CREATE A PLATFORM FOR SENSITIVE DETECTION OF SIGNIFICANT, PHENOTYPE-NEAR BIOMARKERS OF EXPOSURE, HARM AND DISEASE.

It will also create a platform for the detection of signalling pathways in environmental health. HICE concentrates in its initial phase on fresh aerosols because of strong evidence for acute health effects due to fresh combustion related emissions (e.g. from traffic). After the establishment of the HICE consortium, it is aimed at further following the path to translate fundamental scientific environmental health results to human health studies beyond the INF funding period.

This will include additional aspects of aerosol and air pollution-induced diseases. In this respect, the currently controversially discussed questions on the biological activity of aged aerosols, the influence of components of secondary aerosols such as ozone or PAN and the health risks from indoor aerosols are relevant.

Other environmental health aspects addressed on a much longer time scale and with additional partners may include further environmental health effects beyond the effects mediated by the air compartment, e.g. due to nutrition and food or water contamination, skin exposure or effects of climate change (e.g. UV-radiation).

The long-term character of the scientific tasks of HICE is urging us to put a particular emphasis on the building of a permanent research structure, based on the backbone of the cooperation between the Helmholtz Zentrum München and the University of Rostock (e.g. JMSC). Utilising the developed HICE management concepts and network a sustainable added value shall thus be generated.

The structures for governance, interinstitutional cooperation and web-based interdisciplinary education in the HICE concept are capable of associating further scientific partners and may thus serve as a basis for a growing international research network of excellence with a Helmholtz Institute or department as a core.

Joint Mass Spectrometry Centre (JMSC)

THE JMSC IS THE JOINT MASS SPECTROMETRY CENTRE OF THE UNIVERSITY OF ROSTOCK AND THE HELMHOLTZ ZENTRUM MÜNCHEN. IT WAS FOUNDED IN APRIL 2008.

In April 2008, the "Joint Mass Spectrometry Centre", a cooperation of the University of Rostock (UR, Chair of Analytical Chemistry) and the Helmholtz Zentrum München-German Research Center for Environmental Health (HMGU, Cooperation Group Comprehensive Molecular Analytics – CMA) was inaugurated. The Joint Mass Spectrometry Centre (JMSC) is headed by Prof. Dr. Ralf Zimmermann who holds the Chair of Analytical Chemistry at the University of Rostock and directs the Cooperation Group CMA at the Helmholtz Zentrum München.

From top to bottom: Aerial image of the campus of Helmholtz Zentrum München; main building of the University of Rostock.

The JMSC develops and applies novel mass spectrometric and chromatographic techniques and methods for analysis of complex chemical and biological molecular systems relevant for Environmental Health research. The research foci of the JMSC include activities the field of comprehensive on- and off-line analysis of aerosols and gases as well as the characterization of metabolites in living systems (metabolomics). Research topics of the JMSC are structured in three corresponding research areas at UR and HMGU, respectively (Figure 1). The first research area of the JMSC is focused on environmental aspects and their impact on human health. The main objective in the research field "Environmental and Process Analysis" in Rostock is the analysis of chemical signatures of significant technical and environmental processes. Furthermore methods for ultra high resolution mass spectrometry devices are operated and optimised to profile complex molecular mixtures.

The corresponding research field at the HMGU is "Health Relevant Environmental Analysis – Aerosol Research" (HAR). It is embedded in the framework of the HMGU "Environmental Health" POF program and focuses its research activities on ambient aerosols and their health effects. The second research area of the JMSC is concerned with biomedical and health-related applications. One focus of "Biomedical Analysis" in Rostock is the comprehensive analysis of breath gas. The corresponding research area in

Munich is named "Comprehensive Molecular Profiling" (CMP). It develops and applies novel multidimensional profiling techniques for non-targeted metabolic characterisation, for instance in diabetes research or in cell-based toxicological studies on the effect of inhaled aerosols. Moreover, this unit develops statistical data analysis tools for this purpose. The third research area of the JMSC is "Analytical Method Development" (AMD) and is identically named at both institutions. In Rostock the AMD focuses on the advancement and implementation of single and multiphoton ionisation technologies. The photon sources consist of laser or lamp-based light sources, such as electron-beam pumped rare-gas excimer light sources (EBEL).

At the HMGU, re-search is concerned with the development and application of joint analytical systems. Examples include comprehensive two-dimensional gas chromatography and thermogravimetry (TG) coupled to single-photon ionisation time-of-flight mass spectrometry. In 2009 the company "Photonion GmbH" was founded as spin-off of the JMSC with support of the Helmholtz Enterprise Funds program. Photonion is based in Schwerin and at the campus of the Helmholz Zentrum München.

The JMSC contributed to a proposal for a new Research Building, focusing on research on complex molecular systems which was coordinated by the Department Life, Light and Matter of the Interdisciplinary Faculty (INF) of the University of Rostock. The proposal was granted and the new Research building is currently under construction. Furthermore, a new extension building, which will host the rooms of the Chair of Analytical Chemistry, is in the planning phase. The laboratory building at the Helmholtz Zentrum München is under rebuilding and renovations, too. Thus in the near future modern laboratory space will be available for all JMSC co-workers. The concept of Virtual Institute HICE was developed at the JMSC in the aftermath of a workshop which was organised in 2010 at the Analytica Conference 2012 and the Helmholtz Zentrum München (see Analytical and Bio Analytical Chemistry 401 (2011) 3041 ff).

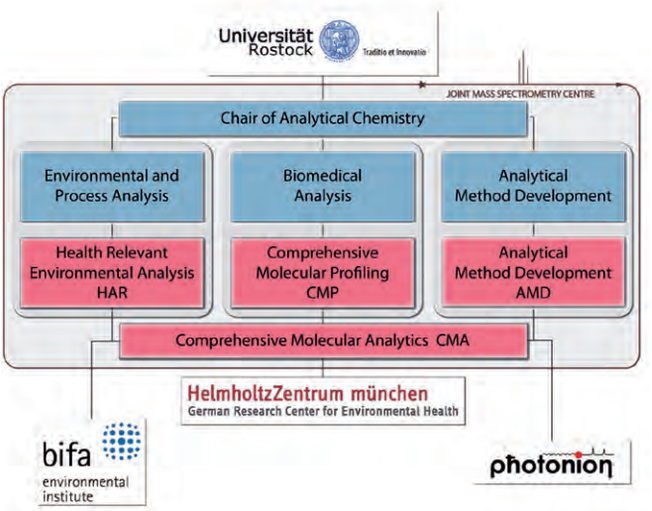


Figure 1: Organisational chart of the Joint Mass Spectrometry Centre (JMSC). The JMSC is divided into three corresponding research areas at the University of Rostock and the Helmholtz Zentrum München that intensely cooperate with each other. The cooperation partner bifa Environmental Institute GmbH and the JMSC spin-off company Photonion GmbH are closely related to research areas 1 and 3 of the JMSC, respectively.

HICE ▸ Aerosols and Health
Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health

HICE Employees

Prof. Dr. Ralf Zimmermann

2012: Spokesperson HICE

2009: Cofounder of "Photonion GmbH"

Since 2008: Full Professor of Analytical Chemistry (Chair), University of Rostock (2008), and Head of the Joint Mass Spectrometry Centre (University of Rostock and Helmholtz Zentrum München)

Since 2008: Head of the cooperation group "Complex Molecular Analytics", Institute of Ecological Chemistry, Helmholtz Zentrum München

2001 - 2008: Director of Chemistry Department, bifa-Institute, Augsburg

2001 - 2008: Associate Professor for Analytical Chemistry (C3), University of Augsburg

1999: Postdoc at the University of Antwerp (Prof. Dr. Adams)

1995 - 2001: Habilitation Technical University of Munich-Weihenstephan (Prof. Dr. Kettrup)

1993 - 1995: PhD work in physical chemistry at the TUM (Prof. Dr. Schlag and Prof. Dr. Kettrup)

1990 - 1993: Pre-Diploma (BSc) in Physics at the Ludwig Maximilian University of Munich

1987 - 1990: Diploma (MSc) and Pre-Diploma (BSc) in Chemistry at the Technische Universität München (TUM)

Key Publications

Hanley L, Zimmermann R; Anal. Chem. 81, 4174-4182 (2009)

Bente M, et al. M. Anal. Chem. 80, 8991-9004 (2008)

Gröger T, et al. J. Chrom. A 1200, 8-16 (2008)

Helmholtz Zentrum München

Laarnie Müller
PhD Student

Sabine Dvorski
PhD Student

Analysis of biological samples and combustion source particulate matter by comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry (GCxGC-TOFMS) and GC high resolution-TOFMS (GC-HRTOFMS) to investigate the impact of aerosols on the metabolism.

Sorana Scholtes
Project Manager HICE

University of Rostock

Sophie Klingbeil
PhD Student
Statistical tools and evaluation.

Johannes Passig
Johannes is developing and applying new photoionisation mass spectrometric techniques for on-line detection of reactive gas phase species in the effluents of combustion engines and bio mass burning.

Literature

1. Dockery, D.W., et al., An association between air pollution and mortality in six U.S. cities. New England Journal of Medicine, 1993. 329(24): p. 1753-1759.

2. Ghio, A.J., Biological effects of Utah Valley ambient air particles in humans: A review. Journal of Aerosol Medicine-Deposition Clearance and Effects in the Lung, 2004. 17(2): p. 157-164.

3. Correa, S.M. and G. Arbilla, Carbonyl emissions in diesel and biodiesel exhaust. Atmospheric Environment, 2008. 42(4): p. 769-775.

4. Gminski, R., T. Tang, and V. Mersch-Sundermann, Cytotoxicity and genotoxicity in human lung epithelial A549 cells caused by airborne volatile organic compounds emitted from pine wood and oriented strand boards. Toxicology Letters, 2010. 196(1): p. 33-41.

5. Cuperlovic-Culf, M., et al., Cell culture metabolomics: applications and future directions. Drug Discov Today, 2010. 15(15-16): p. 610-21.

6. Oldiges, M., et al., Metabolomics: current state and evolving methodologies and tools. Appl Microbiol Biotechnol, 2007. 76(3): p. 495-511.

7. Park, S.J., et al., Global physiological understanding and meta-bolic engineering of microorganisms based on omics studies. Appl Microbiol Biotechnol, 2005. 68(5): p. 567-79.

Comprehensive Pneumology Center (CPC) / Institute of Lung Biology and Disease (iLBD)

THE CPC / iLBD IS A TRANSLATIONAL RESEARCH CENTER DEDICATED TO PULMONARY MEDICINE.

It was founded by three partners: the Helmholtz Zentrum München - German Research Center for Environmental Health (HMGU), the Ludwig-Maximilians-Universität (LMU) with the University Hospital, and the Asklepios Hospital München-Gauting in Germany.

Chronic lung diseases are one of the leading causes of death worldwide; the number of people who die in consequence of a lung disease will increase in the future. However, the research of lung diseases is still at its early stages. Therefore, the overall mission of the CPC/iLBD is to perform cutting edge basic and translational research on chronic lung disease, including chronic obstructive pulmonary disease (COPD), lung cancer, asthma, bronchopulmonary dysplasia (BPD) and pulmonary fibrosis.

The significant contribution of CPC/iLBD to HICE is to offer interventional "proff-of-concept" studies by using animal models for chronic lung disease. This also includes the well characterised cigarette smoke-induced mouse model of COPD. This mouse model provides a unique opportunity to analyse the role of individual pathways for combustion aerosol, particle, and gas phase exposures.

Prof. Dr. Oliver Eickelberg

Oliver Eickelberg is Professor of Medicine at the Ludwig-Maximilians-Universität (LMU), Institute of Experimental Pneumology and Chairman of the Comprehensive Pneumology Center. He is also Director of the Institute of Lung Biology and Disease (iLBD) at the Helmholtz Zentrum München. He has contributed several key studies, which are concerned with the pathogenic role of the TGF-β superfamily in pulmonary arterial hypertension (PAH) and idiopathic lung fibrosis (IPF). His expertise and research interest focuses on lung tissue remodelling, including the interplay of the lung epithelium with the underlying mesenchyme ("epithelial-mesenchymal crosstalk") in chronic lung diseases with distortion of the epithelial-mesenchymal trophic unit (EMTU), particularly interstitial fibrosis and COPD.

Dr. Ali Önder Yildirim

He is the head of the small animal facility (SMAF) that combines the animal models for chronic lung disease at the CPC/iLBD and is deputy director of the iLBD. His focus area is inflammatory lung diseases, in particular cigarette smoke-related COPD. His research group investigates the underlying mechanisms of the development of the disease and tries to identify new therapeutical targets.

Key Publications

Prof. Dr. Oliver Eickelberg

Takenaka S, Möller W, Semmler-Behnke M, Karg E, Wenk A, Schmid O, Stoeger T, Jennen L, Aichler M, Walch A, Pokhrel S, Mädler L, Eickelberg O, Kreyling WG; Efficient internalization and intracellular translocation of inhaled gold nanoparticles in rat alveolar macrophages, Nanomedicine (London, England), [Epub ahead of print] (2012).

Scotton CJ, Krupiczojc MA, Königshoff M, Mercer PF, Lee YC, Kaminski N, Morser J, Post JM, Maher TM, Nicholson AG, Moffatt JD, Laurent GJ, Derian CK, Eickelberg O, Chambers RC; Increased local expression of coagulation factor X contributes to the fibrotic response in human and murine lung injury, The Journal of Clinical Investigation, 119(9), 2550-2563 (2009).

Königshoff M, Kramer M, Balsara N, Wilhelm J, Amarie OV, Jahn A, Rose F, Fink L, Seeger W, Schaefer L, Günther A, Eickelberg O; WNT1-inducible signaling protein-1 mediates pulmonary fibrosis in mice and is upregulated in humans with idiopathic pulmonary fibrosis, The Journal of Clinical Investigation, 119(4), 772-787 (2009).

Dr. Ali Önder Yildirim

Clauss M, Voswinckel R, Rajashekhar G, Sigua NL, Fehrenbach H, Rush NI, Schweitzer KS, Yildirim AÖ, Kamocki K, Fisher AJ, Gu Y, Safadi B, Nikam S, Hubbard WC, Tuder RM, Twigg HL 3rd, Presson RG, Sethi S, Petrache I; Lung endothelial monocyte-activating protein 2 is a mediator of cigarette smoke-induced emphysema in mice, The Journal of Clinical Investigation, 121(6), 2470-2479 (2011).

Yildirim AÖ, Muyal V, John G, Müller B, Seifart C, Fehrenbach H; Palifermin induces alveolar maintenance programs in emphysematous mice, American Journal of Respiratory and Critical Care Medicine, 181(7), 705-717 (2011).

Kneidinger N, Yildirim AÖ, Callegari J, Takenaka S, Stein MM, Dumitrascu R, Bohla A, Bracke KR, Morty RE, Brusselle GG, Schermuly RT, Eickelberg O, Königshoff M; Activation of the WNT/ β -Catenin Pathway Attenuates Experimental Emphysema, American Journal of Respiratory and Critical Care Medicine, 183(6), 723-733 (2010).

Web

www.cpc-munich.org

Institute of Biomathematics and Biometry Helmholtz Zentrum München

THE RESEARCH GROUP STOCHASTIC MODELLING AND STATISTICS IS A RESEARCH UNIT OF THE INSTITUTE OF BIOMATHEMATICS AND BIOMETRY (IBB) OF THE HELMHOLTZ ZENTRUM MÜNCHEN.

This research unit is concerned with probabilistic and statistical modelling, classical statistics, as well as statistical analysis and exploration of data. The emphasis is on biological and medical applications. The group has expertise in mathematics, statistics, as well as time series and image analysis. It consists of scientists with a mathematical, statistical and/or engineering background. There are intimate connections with the analysis, numerical, and computational groups in the IBB, to the experimental institutes at the Helmholtz Zentrum München and also to external institutes, in particular those concerned with genetics, molecular biology and microbiology, pathology and imaging.

Dr. Klaus Hahn

Dr. Hahn has a permanent scientist position at the IBB of the Helmholtz Zentrum München. His main scientific contributions are in the fields of nuclear physics, radiation biology/radiation protection, neuroimaging and neuroscience. After studying theoretical physics at the LMU Munich he obtained his doctoral degree at the University of Tübingen. His contributions cover theoretical, mathematical, numerical and statistical investigations and have led to about 75 refereed papers. He is also engaged in the education of young scientists and co-editor of the International Journal of Biomathematics and Biostatistics.

Key Publications

Hahn K, Prigarin S, Rodenacker K, Hasan K; Denoising for Diffusion Tensor Imaging with low Signal to Noise Ratios: Method and Monte Carlo Validation, International Journal for Biomathematics and Biostatistics, 1(1), 63-81 (2010).

Shao J, Hahn K, Yang Q, Böhm C, Wohlschläger A, Myers N, Plant C; Hierarchical Density-based Clustering of White Matter Tracts in the Human Brain, International Journal of Knowledge Discovery in Bioinformatics, 1(4), 1-26 (2010).

Shao J, Hahn K, Yang Q, Böhm C, Wohlschläger A, Myers N, Plant C; Combining Time Series Similarity with Density-based Clustering to identify Fiber Bundles in the Human Brain, IEEE International Conference on Data Mining, ICDM 2010, 747-754 (2010).

Dr. Hagen Scherb

Hagen Scherb is Mathematician and Biostatistician at the Institute of Biomathematics and Biometry (IBB), Helmholtz Centre Munich, German Research Center for Environmental Health (HMGU). He has long experience in the field of environmental health risk assessment. He is especially interested in mathematical and statistical methods for the analysis of ecological data. He is head of ImStatLab (Image Analysis and Statistics consulting Laboratory) a consulting and service unit intended to serve as an interface between HMGU and external scientists and the diverse IBB groups. This group provides assistance for the solution of practical problems, in particular in image analysis and statistics, but also in other fields of mathematics.

The focus of this unit is on developing image analysis, statistics, and general mathematical methods as an integral part in interdisciplinary research, which requires mathematicians and statisticians to become vital and emancipated partners with subject matter scientists and engineers. Emphasis is on data analysis and data mining under the constraints of variability and uncertainty.

Key Publications

Scherb H, Voigt K; Response to W. Kramer: The human sex odds at birth after the atmospheric atomic bomb tests, after Chernobyl, and in the vicinity of nuclear facilities: comment (doi:10.1007/s11356-011-0644-8), Short Research and Discussion, Environmental Science and Pollution Research, 19 (2012).

Sperling K, Neitzel H, Scherb H; Evidence for an increase in trisomy 21 (Down syndrome) in Europe after the Chernobyl reactor accident, Genetic Epidemiology, 36(1), 48–55 (2012).

Fuß R, Ruth B, Schilling R, Scherb H, Munch JC; Pulse emissions of N2O and CO2 from an arable field depending on fertilization and tillage practice, Agriculture, Ecosystems & Environment, 144(1), 61-68 (2011).

Web

www.helmholtz-muenchen.de/en/ibb

Institute of Epidemiology II Helmholtz Zentrum München

THE INSTITUTE OF EPIDEMIOLOGY II FOCUSES ON THE ASSESSEMENT OF ENVIRONMENTAL AND LIFE STYLE RISK FACTORS THAT JOINTLY AFFECT MAJOR CHRONIC DISEASES SUCH AS DIABETES, HEART DISEASE AND MENTAL HEALTH.

Research builds on the unique resources of the KORA cohort, the KORA myocardial infarction registry and the KORA aerosol measurement station.

Aging-related phenotypes have been added to the KORA research portfolio within the frame of the Research Consortium KORA-Age.

The institute has published internationally acknowledged contributions to the identification of risk factors for cardiovascular diseases and diabetes where inflammatory responses triggered by particulate matter or by psychic stress had played an important role.

The institute's contributions are specifically relevant for the population, as modifiable personal risk factors are being researched that could be influenced by the individual or by improving legislation for the protection of public health.

Prof. Dr. Annette Peters

Prof. Dr. Annette Peters is Director of the Institute of Epdiemiology II, Helmholtz Zentrum München (since 2010).

2008 - 2013: Adjunct Associate Professor at the Department of Environmental Health, Harvard School of Public Health, Boston, USA.

2003 - Present: Privatdozent Epidemiology Ludwig-Maximilians University, Munich, Germany.

2007 - 2010: Head of the Research Units "Epidemiology of Air Pollution Health Effects" and "Epidemiology of Chronic Diseases," Institute of Epidemiology, Helmholtz Zentrum München, Neuherberg, Germany.

2001 - 2007: Head of the Research Unit "Health Effects of Ambient Particles," Institute of Epidemiology, Helmholtz Zentrum München, Neuherberg, Germany.

Web

www.helmholtz-muenchen.de/en/epi2/home

Dr. Josef Cyrys

Exposure assessment of indoor and outdoor air pollutants: Dr. Cyrys's research interest is, in particular, the development and validation of new measurement methods for an improved physical and chemical characterization of particles to meet epidemiological requirements. He is interested in the source apportionment, the spatial and temporal variability of fine and ultrafine particles, as well as in the relationship between indoor, outdoor and personal exposure to particulate air pollution.

Dr. Cyrys is team leader of the research unit "Exposure Assessement" of the Helmholtz Zentrum München, Institute of Epidemiology II, and senior scientist at the Environment Science Center, University of Augsburg.

Web

www.helmholtz-muenchen.de/epi/arbeitsgruppen/epidemiologie-von-luftschadstoffwirkungen/staff-mitarbeiterinnen/cyrys-josef

HICE ▸ Aerosols and Health
Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health

Medical Radiation Physics and Diagnostics Helmholtz Zentrum München

THE RESEARCH UNIT MEDICAL RADIATION PHYSICS AND DIAGNOSTICS (AMSD; DIRECTOR: PROF. DR. CHRISTOPH HOESCHEN) AT THE HMGU ESPECIALLY WORKS ON DOSE REDUCTION STRATEGIES IN MEDICAL IMAGING.

In terms of evaluating new diagnostic approaches and radiation metabolomics the AMSD developed methodologies (principal investigator: Dr. Wilfried Szymczak) to use Proton Transfer Reaction Mass Spectrometry PTR-MS breath gas investigations on humans, head space analyses on mice and on-vitro cells. Breath provides a non-invasive window to metabolic processes as trace molecular biomarkers in the blood partition from the blood stream via the alveolar pulmonary membrane into the lungs. In vitro cells release volatile biomarkers directly at the air liquid interface into the headspace. The molecular profile of breath or headspace reflects changes in metabolic processes brought about by abnormal physiologies and biochemistries, such as those which occur in disease.

The fast on-line mass spectrometric diagnosis tool of PTR-MS has a great potential to characterise the impact of environmental exposure on the metabolism of in vitro cells and animal models. The non-invasive access to the volatile metabolites in breath concurrently extends the investigations on biological effects, e.g. metabolic activity. The head-space in the air-liquid interface (ALI) set-up of cell cultures could be "sniffed" directly during or after the exposure to identify biomarkers in the volatile metabolite spectrum. The fast recording of mass spectra with the PTR-TOF-MS favors non-targeted investigations without restriction in mass and sensitivity.


Prof. Dr. Christoph Hoeschen (left) and Dr. Wilfried Szymczak (right).

Key Publications

Brunner C et al.; Discrimination of cancerous and non-cancerous cell lines by headspace-analysis with PTR-MS, Analytical and Bioanalytical Chemistry, 397(6), 2315-2324 (2010).

Greiter M et al.; Differences in Exhaled Gas Profiles between Patients with Type 2 Diabetes and Healthy Controls, Diabetes Technology & Therapeutics, 12(6), 455-462 (2010).

Fedrigo M, Hoeschen C, Oeh U; Multidimensional statistical analysis of PTR-MS breath samples: A test study on irradiation detection, International Journal of Mass Spectrometry, 295(1-2), 13-20 (2010).

Web

www.helmholtz-muenchen.de/en/amsd

ZAUM - Center for Allergy and Environment

THE CENTER OF ALLERGY & ENVIRONMENT (ZAUM) IS A JOINT CENTER OF THE HELMHOLTZ ZENTRUM MÜNCHEN AND THE TECHNICAL UNIVERSITY MUNICH.

ZAUM conducts environmental and basic clinical research. The aim is to understand environmental diseases such as allergies, to assess risks and to develop preventive interventions as well as therapies for established diseases.

The focus of the ZAUM is allergen tolerance. Basic immunological mechanisms are looked upon from two points of view. First: What happens when immunological tolerance is broken? Second: How can immunological tolerance be recovered? Immunological tolerance is primarily controlled by "memory"-cells, the T and B-lymphocytes. Based on intervention with these cells we expect improved and long-term effective therapies for allergy patients.

Priorities

The translation of our research results into clinical application is our highest priority. Most experiments are performed in humans and with primary human cells or biopsies. A recent success of our investigations on immune memory, specifically the T cell, was recently published in the NEJM (2011 Jul 21;365(3):231-8) and revealed the antagonistic nature of Th2 and Th1/Th17 in the pathogenesis of atopic eczema and psoriasis, respectively. In cooperation with Novartis and the Imperial College London, we initiated a phase II clinical trial to determine whether VAK694 when combined with subcutaneous immunotherapy leads to long-term immune tolerance to allergen in individuals with seasonal allergic rhinitis (NCT01018693). The design of this essay goes back to preliminary work, which was published in Plos Biology in 2007 (Mantel, Plos Biol 2007, 5:12; 2847) and which showed that IL-4 is an effective inhibitor of Treg-induction. By blocking this mechanism, we expect improved therapy effects by the induction of specific allergen tolerance.

Prof. Dr. Jeroen Buters

Jeroen Buters leads the group "Environment", which focuses on the environmental cause of allergies. The group "Environment" mainly investigates how environmental and climatic changes modify the allergenicity of air-borne pollen. Another research topic is the influence of environmental pollution on allergies due to waste products of combustion (fine dust and the organic phase connected to them), and the toxic effects of indoor particulate material from schools. All projects include immunologic effects pivotal in allergies.

Research Projects

The group discovered that pollen have an at least 10-fold biological variability when releasing allergens. This result is important for patients with allergies, because symptoms depend on the quantity of the allergen. For the comprehensive investigation of this important correlation, a pan-European project was initiated in order to classify the most common released allergens. The aim, in the interest of the patient, is to develop an early warning system (www.HIALINE.com). This project is sponsored by the European Union. The investigation of anthropogenic agents of combustion (i.e. diesel engine exhaust particles) and their influence on the human immune system is a further project, which is of special relevance for our urbanised environment. Combustion products occur mainly outdoors.Indoor particles are important as well because most individuals stay indoors more than 90 % of their time. Our observation is that the indoor fine dust contamination is much higher than outdoors, and that indoor particles (PM10) are toxicologically at least if not more active than outdoor air particles. At present, we analyse the toxicologic impact of airborne particles from elementary schools. The risk deriving from these dusts is presently uncertain.

Our organism is not defenseless against environmental agents, but metabolises these chemical agents. Ironically, agents can be generated that are sometimes more toxic than the mother agent. The group integrates the role of these metabolising enzymes and therefore allows preventative measures.

Dr. Sebastian Öder

Dr. Öder obtained his PhD in 2011 at the Technical University Munich on the subject "toxicity of particulate matter from school indoor air". The systems used for his thesis are well suited for testing the materials generated in HICE. In addition, Dr. Öder will focus on the allergy-related effects of combustion products. Dr. Öder is currently training to become a registered toxicologist (Fachtoxikologe).

Key Publications

Buters JTM and the HIALINE working group; Release of Bet v 1 from birch pollen from 5 European countries, Results from the HIALINE study, Atmospheric Environment, in press (2012).

Oeder S, Dietrich S, Weichenmeier I, Schober W, Pusch G, Jorres RA, Schierl R, Nowak D, Fromme H, Behrendt H, Buters JT; Toxicity and elemental composition of particulate matter from outdoor and indoor air of elementary schools in Munich, Germany, Indoor Air, 22(2), 148-158 (2012).

Zirbs M, Purner C, Buters JT, Effner R, Weidinger S, Ring J, Eberlein B; Gstm1, GstT1 and GstP1 gene polymorphism in polymorphous light eruption, Journal of the European Academy of Dermatology and Venereology (2012).

Web

www.zaum-online.de
www.hialine.com

Department of Piston Engines and Internal Combustion Engines, University of Rostock

THE DEPARTMENT OF PISTON ENGINES AND INTERNAL COMBUSTION ENGINES WAS FILLED WITH THE CURRENT CHAIR PROF. DR.-ING. HORST HARNDORF IN 2006.

The goal was to focus research attention more closely on more traditional strengths of the department, such as research on the use of alternative fuels in internal combustion engines, laser optical injection spray analysis and the analysis of emission-reducing measures for large-and marine diesel engines and to combine these with the current work on developing combustion processes, exhaust after treatment and development of thermodynamically based control algorithms for future engine.

The research activities of the Department are focused on the optimization of energy processes in internal combustion engines and exhaust after-treatment as well as the adaptation of engines to alternative gaseous and liquid fuels. The following major research areas are dealt with:

- Analysis of combustion processes in gasoline and diesel engines to gain a better understanding of combustion processes, heat transfer and charge air motion processes in internal combustion engines.
- Modeling of the combustion process in internal combustion engines, creation and verification of related thermodynamic-kinetic models to predict pollutant emissions from gasoline and diesel engines.
- Combustion optimization of heavy fuel oil fired marine engines by means of time-and stroke-controlled injection systems.
- Optimization of engine measurement instrumentations and extension of the interpretation.
- Analysis, modeling and optimization of thermo-and fluid-dynamic processes in the charge air and exhaust lines of engines.
- Studies of the injection characteristics of standard and alternative fuels, analysis of jet breakup, the beam propagation and the air inlet of the jet, derivation of optimization concepts.
- Research on the adaptation of engines to renewable fuels by fuel-specific optimization of the injection, the engine control unit data and the fuel system.
- Field test of engines that run on renewable fuels in particular for use in agriculture and in Combined heat and power-units.

Prof. Dr. Horst Harndorf

holds the chair of Combustion Engines. He has more than 25 years experience in R&D in this area, automotive operation and applica-

tion of alternative fuels in engines, including ~15 years in industry with Robert-Bosch GmbH in a management position before he was appointed professor at the University of Rostock. Beside his lectures at the University of Rostock, he leads several research projects covering exhaust treatment, fuel-mixture generation, heat transfer, tribilogical problems and application of alternative sustainable fuels (natural gas, bio gas, dimethylether, bio fuels, etc.).

Dr. Ulrike Schümann

Head of the laboratory for fuels and Lubricants. She supervises several projects concerning influences of alternative sustainable fuels on lubricating oil as well as the influence of fuel blends on the operating behaviour of modern diesel engines. Furthermore she deals with fuel characteristics under extreme conditions. Besides her work at the University of Rostock she is active in several specification organisations and biofuel networks.

Dr.-Ing. Christian Fink

Head of the work group for injection systems and fuel-mixture generation. He studies the impact of common rail injection systems on engine emissions and fuel consumption for several fuels (e.g. diesel blends, heavy fuel oil). Therefore, jet spreading and nebulisation is analysed in a high pressure-high temperature injection chamber and at an engine test-bed by optical and laser optical methods.

Dipl.-Ing. Benjamin Stengel

Research assistant at the Chair of Piston Machines and Combustion Engines. He coordinates and organises HICE-related engine measurement campaigns involving different combustion processes and fuels at the University of Rostock. Moreover, he deals with exhaust sampling and measurement methods in order to achieve comparable results.

Key Publications

Schümann U, Berndt S, Harndorf H, Malicki D; In-service behaviour of lubricating oil in biodiesel and plant oil operation, 8th International Colloquium Fuels, Conventional an Future Energy for Automobiles, Stuttgart/ Ostfildern, 19-20 January (2011).

Schümann U et al.; Bestimmung des Pflanzenölanteils in gebrauchten Dieselmotorenölen - Motorische Auswirkungen und verfügbare Analysenverfahren, Tribologie und Schmierungstechnik, Heft 04 - 2010, Expert Verlag, Juli-August (2010).

Harndorf H, Schümann U, Wichmann V, Fink C; Motorprozessverhalten und Abgasemissionen alternativer Kraftstoffe im Vergleich mit Dieselkraftstoff, Motortechnische Zeitschrift 7-8, 640-646, ISSN 0024-8525 10814, Juli-August (2008).

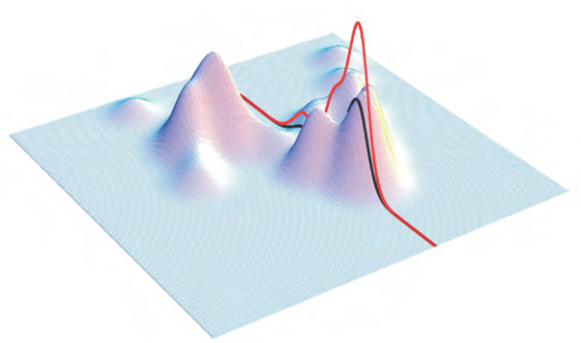
Web

www.lkv.uni-rostock.de/en

Department of Systems Biology and Bioinformatics, University of Rostock

THE DEPARTMENT OF SYSTEMS BIOLOGY AND BIOINFORMATICS OF THE UNIVERSITY OF ROSTOCK FOCUSES ON THE DEVELOPMENT OF SYSTEMS AND CONTROL METHODOLOGIES USING MATHEMATICAL MODELLING AND STATISTICAL DATA ANALYSIS APPLIED TO COMPLEX DYNAMICAL SYSTEMS.

We build realistic and useful models of biological phenomena from the molecular level, to cellular, tissue and organismal levels through close collaborations with experimental biologists. Our current projects range from cancer research and aging research to the development of methods for stochastic modelling.



Our contribution to HICE is the expertise in mathematical modelling and the description of complex molecular systems. This includes the development of bioinformatics tools and statistical data analysis.

Prof. Dr. Olaf Wolkenhauer

His research interest is in data analysis and mathematical modelling directed towards an understanding of cell function. He received his first degrees in control engineering in 1994 and obtained his PhD from the University of Manchester in 1997 for research on the application of possibility theory to data analysis. Following a research lectureship at the Control Systems Centre at Manchester and a research fellowship at the Technical University Delft in the Netherlands, he moved to the University of Rostock in Germany in 2003. There he holds the Chair in Systems Biology and Bioinformatics. Since 2005, he has been a fellow of the Stellenbosch Institute for Advanced Study (STIAS) and an Adjunct Professor at Case Western Reserve University, Cleveland, USA.

Key Publications

Ullah M, Wolkenhauer O; Stochastic Approaches for Systems Biology, Springer, ISBN-10: 1461404770 (2011).

Wolkenhauer O, Shibata D, Mesarovic MD; A stem cell niche dominance theorem, BMC Systems Biology, 5(4) (2011).

Rateitschak K, Wolkenhauer O; Thresholds in transient dynamics of signal transduction pathways, Journal of Theoretical Biology, 264(2), 334-346 (2010).

Web

www.sbi.uni-rostock.de/home

Institute of Physics University of Rostock

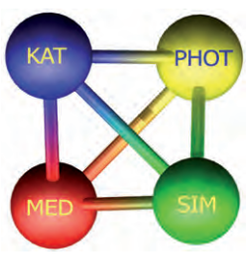
FINITE SIZE, LARGE SURFACE FRACTION, LIMITED CAPACITY FOR HEAT AND CHARGE, AND DISCRETE ELECTRON STATES: THESE ARE THE CHARACTERISTICS OF METAL CLUSTERS AND NANOPARTICLES, ADDRESSED IN THE FIELD OF CLUSTER PHYSICS.

Clusters and Nanostructures at the Institute of Physics, Rostock University

Prof. Dr. Karl-Heinz Meiwes-Broer
PD Dr. Josef Tiggesbäumker
Dr. Viola von Oeynhausen
Dr. Ingo Barke
Dr. Steffen Fiedler

Our research is aimed at the remarkable consequences, many of which are accessible by spectroscopic means. Free clusters in a beam allow for the investigation of the pure cluster properties where the coupling to the environment may be neglected. When deposited onto a surface the cluster-substrate interaction becomes crucial and is a topic of intense research. The experimental methods comprise a manifold of mass spectroscopic techniques, in order to analyze cluster sizes, to mass-select clusters and nanoparticles in a beam, or as detection tool in linear as well as non-linear laser spectroscopy. Besides different ns laser systems the group uses femtosecond lasers, including pulse shaping and colored double pulse techniques. For high photon energies the free electron laser FLASH in Hamburg can be employed.

A large part of the research is conducted within the Sonderforschungsbereich SFB 652, different BMBF projects, and as part of the excellence programs "Light to Hydrogen"and "REMEDIS". Within HICE the group will be involved in the development of photoionisation techniques. This includes the implementation of supersonic nozzle beams together with novel light sources. We may note that our HICE work fits well into the activities of the Department Life, Light and Matter at the Rostock University. The department aims at interdisciplinary research and training in the fields photon sciences, engineering and catalysis, regenerative medicine and numerical simulations. The program comprises science within several faculties and institutes of the Rostock University.



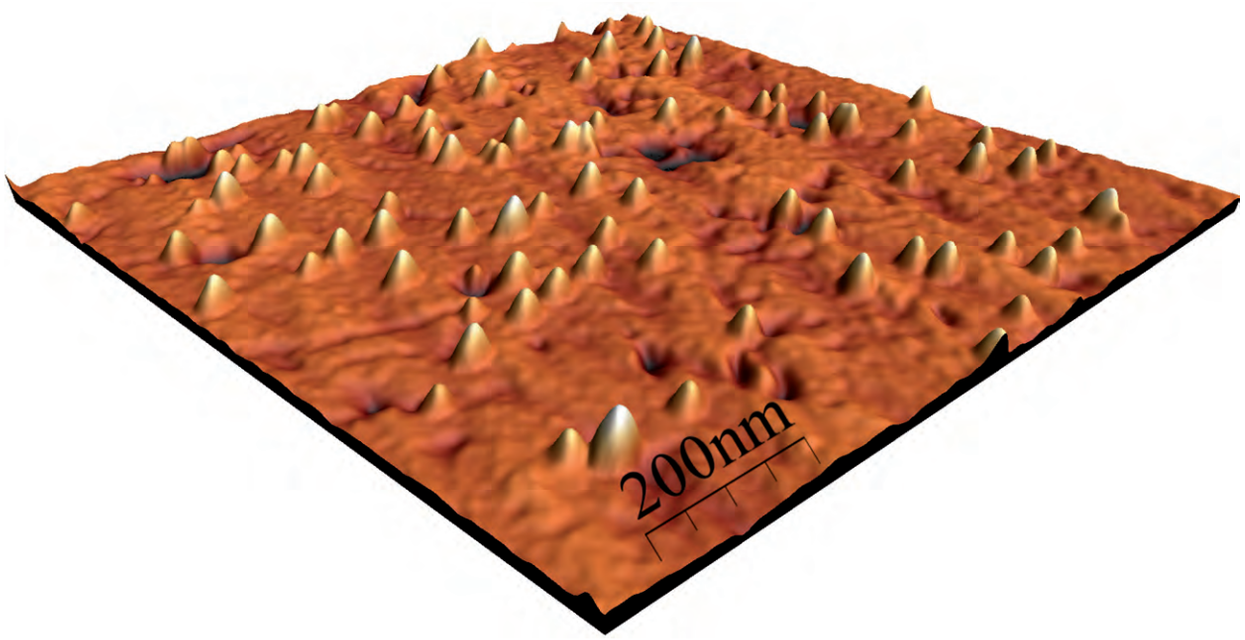
Selected Topics of the Group Clusters and Nanostructures

1. Spectroscopy on Metal Clusters Embedded in Helium Droplets

Ultracold helium nanodroplets provide an interesting superfluid matrix for studies on embedded clusters. The technique of atom pick-up in helium droplets provides a flexible tool to nearly independently adjust the size of both the droplets and the embedded species. For spectroscopy studies, resonant

two photon ionisation is applied to mass-select the embedded neutral metal clusters. In combination with photoelectron spectroscopy, the intermediate state dynamics is

short wavelength radiation up to the x-ray regime. In contrast to atomic gas targets, the temporal laser pulse structure plays a significant role. Stretched and double pulses



Atomic force image of deposited mass-selected silver clusters produced in a magnetron sputtering source.

to be analyzed. Moreover, exotic species like molecular chains or foam-like structures can be generated. In femtosecond pump-probe studies the formation dynamics of metal ion helium snowballs provides information about the local atomic environment.

2. Strong Field Excitations of Molecules and Clusters in the Optical Regime

Intense femtosecond laser pulses are used to investigate strong-field induced phenomena in small particles. Clusters serve as model systems to interrogate multi-electron dynamics relevant for many areas of intense laser matter research, e.g., laser-driven particle acceleration or ultrashort x-ray sources. The many-body aspects of finite-sized objects introduce a special behaviour of the cluster response, as is reflected by the observation of energetic MeV ions, fast keV electrons and

are much more effective in the generation of these energetic species than ultrashort single pulses. Due to the resonant interaction of the oscillating laser field with the collective mode of cluster electrons, an effective acceleration of electrons can be achieved. Recently we could show that adapted light fields (temporally shaped in amplitude and phase) allow the adjustment of the ionic charge state distribution from strong-field cluster interactions nearly at will.

3. Clusters Excited by XUV-light from Free Electron Lasers (FEL)

The rapid advances in the FEL technology have opened new avenues to drive, control, and analyse the structure and dynamics of matter. Several novel approaches, such as single-shot coherent diffractive imaging or ultrafast time-resolved holography of na-

nostructures, small particles, or biological samples are presently in reach or have been demonstrated. A crucial fundamental question being closely related to all existing and upcoming applications of intense FEL light is how the interaction mechanism of intense laser fields with matter develops in the spectral range from the extreme ultraviolet (XUV) up to the x-ray domain. Atomic clusters are an ideal testing ground for corresponding fundamental studies as great experience in their experimental and theoretical analysis is available. The group is involved in several experiments at FLASH in Hamburg.

4. Clusters and Atomic Chains at Surfaces

The properties of nanoclusters typically change substantially compared to the gas phase when brought into contact with surfaces. In view of potential applications a holistic understanding of the cluster-surface system is inevitable. Our group has experience in generating clusters and nanoparticles with physical methods (sputtering, gas aggregation, laser vaporization, arc discharge, helium pick-up). After beam formation, the systems can be mass-selected and deposited onto surfaces. Topics of interest are, e.g., nanomagnetism, or the role of clusters as catalysts. Special interest is devoted to atomic chains, i.e. one-dimensional quantum systems at surfaces. The strongly anisotropic Au-induced reconstruction on silicon can be viewed as the ultimate nanowire. We use those to investigate the physics of electrons in one dimension by scanning tunneling spectroscopy. The results open new routes for quantitative and local control of electron states in metallic nanostructures on the atomic scale.

Key Publications

Polei S, Barke I, Erwin S, Meiwes-Broer KH; Periodic variations in the local surface potential of Si(111)- (5x2)-Au, Physical Review B, 85, 165414 (2012).

Bostedt C, Eremina E, Rupp D, Adolph M, Thomas H, Hoener M, Möller T, de Castro ARB, Tiggesbäumker J, Meiwes-Broer KH, Laarmann T, Wabnitz H, Plönjes E, Treusch R, Schneider JR, Möller T; Ultrafast x-ray scattering of xenon nanoparticles, Imaging transient states of matter, Physical Review Letters, 108, 093401 (2012).

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Web

web.physik.uni-rostock.de/cluster

Karlsruhe Institute of Technology

KARLSRUHE INSTITUTE OF TECHNOLOGY (KIT) IS A HIGHER EDUCATION AND RESEARCH INSTITUTION WITH ABOUT 8900 EMPLOYEES, 21000 STUDENTS AND AN ANNUAL BUDGET OF 750 MILLION EUROS.

KIT was established on October 1, 2009, as a merger of the University of Karlsruhe (founded in 1825), one of Germany's leading research universities, and Forschungszentrum Karlsruhe (founded in 1956), one of the largest research centres of the Helmholtz Association.

Higher education, research and innovation are the three pillars of KIT's activities. KIT's research profile is characterised by a strong focus on energy technology, nanotechnology and materials research, elementary particle and astroparticle physics as well as climate and environmental research. It has significant competencies in the fields of information and communication technologies, mobility systems, optics and photonics, and the interrelations of humans and technology.

KIT will be involved in HICE with its Institute for Technical Chemistry (ITC) and its Institute for Toxicology and Genetics (ITG).

Institute for Technical Chemistry

The activities of ITC (Head: Prof. Dr.-Ing. H. Seifert) are focused on the development of eco-efficient thermal process technologies for the utilisation of biomass, refuse-derived fuels and alternative fuels in high temperature processes. Technologies like combustion, pyrolysis and gasification and reduction technologies for gaseous and particle-based pollutions will be employed. The processes will be applied to power plants, the chemical industry and basic materials industry and the production of transport fuels (bioliq® process). The experimental research activities comprise basic lab scale investigations, applied research at semi-industrial scale and industrial scale facilities. Model based work complements the research activities. The application oriented research will be ensured with the operation of different pilot plants like the grid fired combustion system (TAMARA), the power plant combustion chamber (BRENDA), the hot gas cleaning systems within the flue gas of the rotary kiln based pyrolysis plant and the atmospheric gasification reactor (REGA) as well as for research activities concerning aerosols (AEOLA).

In the **Department Aerosol- and Particle Technology (Head: Dr. H.-R. Paur)** the whole life cycle of airborne particles is being studied. Topics are:

- The formation of nanoparticles in high-temperature processes and microwave plasma is measured by a novel particle mass spectrometer. Model calculations are developed and validated by these experimental data.
- To remove fine particles from combus-

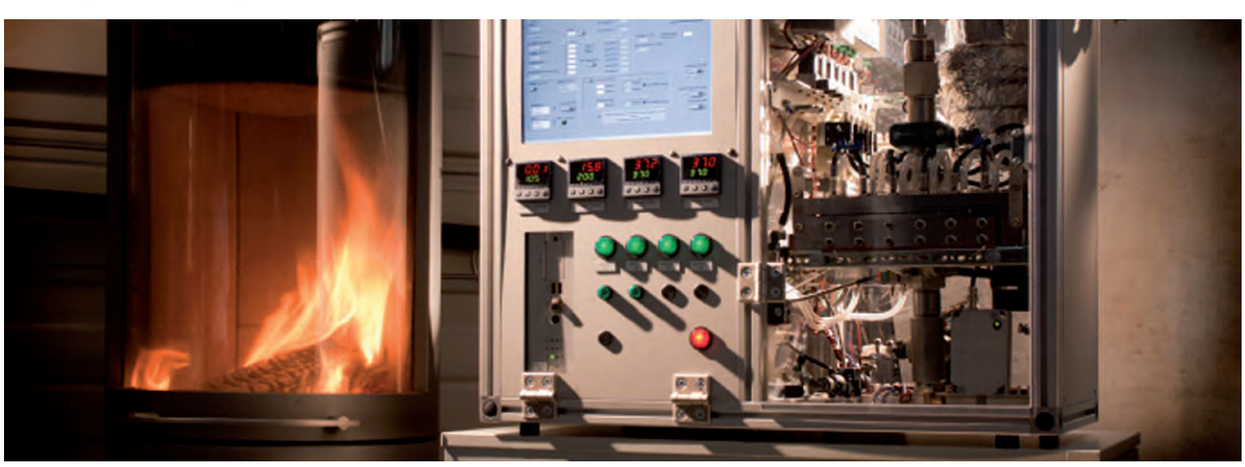
tion, pyrolysis and gasification novel electrostatic precipitators are developed in fundamental studies. The CAROLA®-Electrostatic Precipitators clean offgas from industrial incinerators and from residential wood combustion.

- To quantify and reduce the emission of toxic trace metals from thermal processes we develop measurement systems and gas cleaning processes. The MercOx®-process cleans the flue gas from hazardous waste incinerators.
- To assess the toxicity of nanoparticles and pollutants from biomass combustions, the "Karlsruhe Exposure System" (see the image below) was developed. Reproducible amounts of nanoparticles are sampled from emission sources and deposited onto biological interfaces (lung cells, bacteria).

Institute for Toxicology and Genetics

Research at the ITG (Head: Prof. Dr. U. Strähle) focuses on the elucidation of molecular and cellular interactions at functional interfaces. A major aim is the identification of molecules that play key roles in cellular signaling, in differentiation and proliferation, during embryonic development, and under pathophysiological conditions. Further topics cover proteomics, genomics and molecular toxicology. Through close cooperation with chemists and physicists, these new findings will be used to guide the rational design of new tools for controlling the behaviour of cells in vivo and in vitro. These tools include for example pharmacological substances, so-called "smart drugs" and biofunctionalised surfaces for the cultivation of stem cells.

In the **research group Molecular Toxicology (Head: PD Dr. C. Weiss)** different in vitro systems are used to study the toxicity of nanomaterials and particles from combustion processes. These studies are performed under submerged (cells are covered with medium) as well as at the air-liquid interphase (ALI) to simulate the processes during inhalation of nanomaterials and combustion aerosols. Mechanisms of toxicological responses are also studied using high-throughput/content microscopy and by applying inhibitors and siRNA. Exposure experiments under ALI conditions for the in-vitro assessment of nanoparticle or combustion aerosol toxicity in the human lung cells are operated in close co-operation with the KIT-ITC, where ITG provides the test cells and analyses the biological response.



Compact Karlsruhe Exposure System used to assess the toxictiy of nanoparticles and pollutants from biomass combustion. Image source: KIT.

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KIT Contributions to HICE

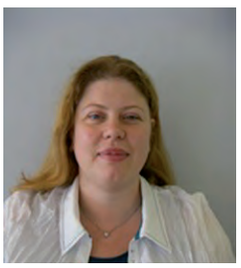
KIT-ITC contributes to WP I by generation and characterisation of test combustion aerosols (from wood combustion) as well as characterisation of combustion aerosols during experimental campaigns. The aerosols are characterised by size distributions and number and mass concentration. The aerosols are provided for the exposure of cell and tissue cultures (see WP 2) using a novel and unique mobile system for exposure of cell cultures at the air-liquid interface, which has been developed at ITC together with Vitrocell. KIT-ITC has planned a next generation exposure system adapted to the requirements of HICE which will be built by ITC in cooperation with Vitrocell supplying especially designed exposure chambers. This HICE exposure system will be used during the experimental campaigns at different sites and emissions sources.

Human and animal lung cell cultures as well as a differentiated multi cell-type human lung tissue model from UCA are facilitated and supervised by KIT-ITG. The biological effects of the respective exposures are monitored by toxicological tests. The examined biological endpoints are cytotoxicity, metabolic activity, cellular functions (e.g. metabolism of foreign substances), oxidative stress and inflammatory response markers. The exposed test cells are also processed for further analyses in WP III (proteome, metabolome). Data are evaluated in cooperation with WP IV.

Dr. Silvia Diabaté

Research interest: Toxicology of ultrafine and nanoparticles.

Sonja Mülhopt, Dipl.-Ing. (BA)



Research interest: Exposure system.

Marco Dilger

After finishing his diploma in food chemistry, he started as a joint PhD student of KIT-ITG and KIT-ITC in March 2012. The goal of his PhD thesis is the in vitro characterization of adverse health effects of anthropogenic aerosols. His main tasks in HICE will be a) exposure of test cell cultures at the air-liquid interface, and b) investigation of the toxicological endpoints thereof.

Key Publications

Mätzing H, Baumann W, Bockhorn H, Paur HR, Seifert H; Detection of electrically charged soot particles in laminar premixed flames, Combustion and Flame, 159(3), 1082-1089 (2012).

Paur HR, Cassee FR, Teeguarden J, Fissan H, Diabate S, Aufderheide M, Kreyling WG, Hänninen O, Kasper G, Riediker M, Rothen-Rutishauser B, Schmid O; In-vitro cell exposure studies for the assessment of nanoparticle toxicity in the lung - A dialogue between aerosol science and biology, Journal of Aerosol Science, 42(10), 668-692 (2011).

Mülhopt S, Paur HR, Diabaté S, Krug HF; In vitro testing of inhalable fly ash at the air liquid interface, In Y.J. Kim & U. Platt (Eds.), Advanced Environmental Monitoring, Springer Netherlands, Dordrecht, 4, 402-414 (2008).

Web

www.kit.edu

Max Delbrück Center for Molecular Medicine Berlin-Buch

THE MAX DELBRÜCK CENTER (MDC) FOR MOLECULAR MEDICINE IS A MAJOR BIOMEDICAL RESEARCH INSTITUTE LOCATED IN THE NORTHEASTERN CORNER OF BERLIN, GERMANY.

The MDC was founded in 1992 with the mission of translating discoveries from molecular research into applications to improve the prevention, diagnosis, and treatment of major human diseases. The site in Berlin-Buch, home to hospital clinics, research institutes and a flourishing biotech industry, is fertile ground for interdisciplinary and patient-oriented research. As a testament to its success, the MDC has been ranked 14th in the Thompson Reuters list of the world's 20 best research institutes for molecular biology and genetics, based on our publication record, the only German research institute on the list.

Currently about 1400 staff members and guests work at the MDC. The work of the MDC's 57 research groups centers around three classes of disease which have an enormous impact on society:

- Cardiovascular and metabolic diseases
- Cancer
- Nervous system disorders

Translational research, bringing the latest science from the bench to the bedside, is carried out within the framework of the Experimental and Clinical Research Center (ECRC) – the centerpiece of our collaborations with the Charité-Universitätsmedizin. The ECRC combines research labs and several outpatient clinics, clinical training programs, and offers funding for groups and specific translational projects, enabling close collaboration between MDC researchers and clinical scientists of the Charité.

The MDC has placed a special emphasis on systems biology, and a major unit called the Berlin Institute for Medical Systems Biology (BIMSB) has been established to pursue this topic in close collaboration with existing groups. The scientific focus of BIMSB is post-transcriptional gene regulation with a particular emphasis on the role of microRNAs in health and disease. Work at the institute is supported by high-throughput technology platforms for mass spectrometry, flow cytometry, confocal and two-photon microscopy, electron microscopy and magnetic resonance tomography, along with bioinformatics services and advanced data modeling, for example mathematical cell physiology.

With over 300 PhD students in several graduate programs, the MDC is helping to educate a new generation of scientists.

The MDC as a collaborating partner in the HICE consortium will contribute its expertise in large scale proteomics. This will fill the gap between transcriptional regulation and the metabolomic and aerosole analysis data.

Dr. Gunnar Dittmar

Dr. Dittmar leads the group for mass spectrometry based proteomics at Max-Delbrück Center for Molecular Medicine. As the central hub for mass spectrometry the Dittmar group interacts with most of the research groups of the MDC and provides proteomic analysis. The spectrum of proteomic techniques includes quantitative shot-gun as well as targeted proteomics. The shot-gun technology combined with the SILAC technology (stable isotope labeling in cell culture) allows the identification and quantification of several thousand proteins in one experiment. This is the basis of proteomic analysis and comparison of different cell populations. Additionally this technique allows the identification of post-translational modifications, which can act as molecular switches to change the function of proteins in a cellular context.

The mapping of post-translational modifications on the transcriptional activator C/EBP is an example of such a collaboration project which lead to the surprising identification of more than 70 modifications present on this regulatory molecule (Leutz et al., 2011). Contrary to the shot-gun approach targeted proteomics focuses on a limited number of proteins. This concentration on less comes with a gain in sensitivity. This allows to detect proteins in very low concentrations. In a collaboration with the Scheidereit and the Wolf group targeted mass spectrometry was applied to the NFkB system.

Protein Degradation

Protein synthesis and degradation are important for the cellular homeostasis and regulatory events. The cell has several mechanisms to selectively degrade proteins, which are tightly controlled. One of these cellular degradation systems is the ubiquitin-proteasome system. The small protein ubiquitin acts as a degradation signal which is covalently attached to the target protein by an enzymatic cascade. Understanding the impact of ubiquitin-mediated degradation on proteomic level is one of the goals of the Dittmar lab.

Tamara Kanashova

She studied biotechnology at the Otto von Guericke university in Magdeburg (Germany). She finished her studies with a diploma thesis, which she prepared in collaboration with a biotechnology company (AnaTox GmbH & Co KG) on quality control procedures for a dissolution sampler. At the end of January she joined the Dittmar group to work on the characterization of proteomic changes in a aerosol exposed cells.

Key Publications

Leutz A, Pless O, Lappe M, Dittmar G, Kowenz-Leutz E; Crosstalk between phosphorylation and multi-site arginine/lysine methylation in C/EBPs, Transcription, 2(1), 3–8 (2011).

Pless O, Kowenz-Leutz E, Dittmar G, Leutz A; A differential proteome screening system for post-translational modification-dependent transcription factor interactions, Nature Protocols, 6(3), 359–364 (2011).

Schwanhäusser B et al.; Global quantification of mammalian gene expression control, Nature, 473, 337–342 (2011).

Web

mdc.helmholtz.de/en

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University of Luxembourg

THE UNIVERSITY OF LUXEMBOURG, FOUNDED IN 2003, IS ONE OF THE YOUNGEST UNIVERSITIES IN EUROPE. IT IS A RESEARCH-FOCUSED UNIVERSITY WITH ABOUT 5000 INTERNATIONAL STUDENTS.

Systems biomedicine has been identified as a high priority research area. For this purpose, the government of Luxembourg has launched a major program in personalised medicine, which includes the establishment of a Centre for Systems Biomedicine (LCSB). Rudi Balling was recruited as the founding director of this new Centre in 2009.

Within the University of Luxembourg, the Luxembourg Centre for Systems Biomedicine (LCSB) is one of two Interdisciplinary Centres. The focus of the LCSB is on understanding the molecular and cellular mechanisms underlying the development and progression of neurodegenerative diseases through experimental and systems biology approaches. Mathematical descriptions of disease relevant networks are developed and used for the modeling and simulation of how diseases develop and how diseases are influenced by genetic predisposition or by external environmental parameters, such as toxic compounds, drugs, nutrition or life style.

Scientists at the LCSB have intensive know-how in studying complex biological systems, particularly in disease network inference and analysis. The staff consists of a highly interdisciplinary team of biologists, MD's, theoretical physicists, computer scientists and engineers trained in systems control and artificial intelligence. Members of the LCSB also have wide expertise in the analysis of the molecular and cellular mechanisms of disease pathogenesis and animal models human diseases.

Metabolomics Group

The metabolomics group at LCSB focuses its research on deciphering the details of cellular metabolism. We are interested in identifying new metabolic pathways and in understanding their functions. Combining wet-lab experiments with bioinformatics and software development, we established a state of the art mass-spectrometry based metabolomics platform.

Standard metabolomics analyses only provide information about metabolite amounts but do not consider metabolic dynamics like me-

tabolic fluxes or enzyme activities. To overcome these limitations, we developed specific stable-isotope based technologies including algorithms and software for the analysis of the dynamics of cellular metabolism.

Metabolomics Platform

Dr. Karsten Hiller

Currently, we routinely analyse intra- and extracellular metabolites in mammalian cells in culture (~100,000 cells), tissue (10 mg) or body fluids like plasma, CSF or urine (5 µl). We developed experimental protocols to efficiently extract small-molecules from the samples and to prepare them for mass-spectrometric measurement. To analyse the recorded complex raw data, we develop required algorithms and implement those in software tools. Until now, the metabolomics group has developed and applied the software MetaboliteDetector and an R based statistical analysis pipeline.

For a more detailed understanding of cellular metabolism, we develop and apply tools based on stable-isotope tracers. Our group established a technology to determine the metabolic fate of a stable-isotope labeled metabolic precursor: The Non-targeted Tracer Fate Detection (NTFD) system detects all compounds downstream of the tracer without any a priori knowledge.

Contribution to HICE

Our contributions to the research objectives of HICE are:

- Discovery: Our stable-isotope assisted and non-targeted technologies allow for the identification of unknown metabolic mechanism induced by exposure to aerosols.
- Validation: Using stable isotopic metabolic precursors we can determine what biochemical reactions are active in a biological system, by verifying the occurrence of stable-isotopes in metabolites downstream of the precursor. Metabolic flux analysis allows for the determination of quantitative data on enzyme activities. This information are required for parameterising and curating systems-level models describing cellular effects induced by aerosols
- Biomarker discovery: Our non-targeted metabolomics measurements provide complex data helping to generate hypothesis and to discover metabolic biomarkers specific for aerosol induced effects.
- Quantitative analysis: Our mass-spectrometric platform provides quantitative measurements of selected metabolites like organic or amino acids in tissues, cells or body fluids. These measurements are essential for hypothesis validation or modeling.

Key Publications

Hiller K, Metallo C, Stephanopoulos G; Elucidation of cellular metabolism via metabolomics and stable-isotope assisted metabolomics, Current Pharmaceutical Biotechnology, 12(7), 1075-1086 (2011).

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Hiller K, Hangebrauk J, Jäger C, Spura J, Schreiber K, Schomburg D; MetaboliteDetector: comprehensive analysis tool for targeted and nontargeted GC/MS based metabolome analysis, Analytical Chemistry, 81(9), 3429–3439 (2009).

Web

wwwde.uni.lu/lcsb

HICE › Aerosols and Health
Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health

University of Eastern Finland

THE UNIVERSITY OF EASTERN FINLAND IS A MULTIDISCIPLINARY UNIVERSITY THAT IS INTERNATIONALLY RECOGNISED FOR ITS COMPETITIVE RESEARCH AND EDUCATION.

The university has four faculties: the Philosophical Faculty, the Faculty of Science and Forestry, the Faculty of Health Sciences, and the Faculty of Social Sciences and Business Studies. With approximately 14000 students and 3000 staff members, it is one of the largest universities in Finland.

Inhalation Toxicology Laboratory, Department of Environmental Sciences, Kuopio, Finland

Thematically, research of the inhalation toxicology laboratory is concentrated on the three leading environmental health problems in the developed world:

1. Outdoor fine particle air pollution
2. Microbial exposures in water damaged buildings
3. Increased incidence of asthma and allergies

The overall aim is to identify the actual causes of adverse health effects associated with these indoor and/or outdoor air pollutants by using cell lines, primary cells (e.g clinical samples), and experimental animals.

Research in the Inhalation Toxicology Laboratory is carried out focusing on:

Activation of immunotoxicological mechanisms of adverse health effects induced by:

1. Source specific combustion emissions
2. Complex mixture of urban air particulate matter
3. Diverse population of indoor air microbes and their toxins

Protective role of environmental microbes: Beneficial effects of environmental microbial exposure on the maturation of immune responses and development of asthma and allergies in early life

The open questions concerning causality between exposure and related health impacts can only be addressed in a multidisciplinary experimental environment which makes possible the analysis of the whole chain from emission source via dilution and transformation to health-related toxicological responses in cells and animals. In order to respond to these challenges, the laboratory has close multidisciplinary collaborations with experts in exposure assessment, combustion technology, environmental technology, aerosol physics and epidemiology. Toxicological research is carried out using particles from various combustion processes, engine emissions and nanoparticles. Research covers studies on proposed toxic mechanisms behind PM-induced adverse health effects including cytotoxicity, inflammation, oxidative stress and genotoxicity.

The laboratory has excellent facilities for toxicological studies, including secondary and primary cell culture laboratories, an exposure and analysis laboratory with latest analysing techniques, a cell culture laboratory for air liquid interface, and a controlled weighing room for the sampling materials. Toxicological endpoints can be analysed with a variety of equipments. Inflammation is analysed with a novel multiplexing device (Sector Imager 2400, MSD technologies, Gaithersburg, MD). Cytotoxicity and oxidative stress can be analysed with a flow cytometer (CyAn, Beckman-Coulter), multilabel counter (Victor3, PerkinElmer) or with an epifluorescence microscopy (Axio Observer Z1, Zeiss).

The Inhalation Toxicology Laboratory staff includes 15 members: a professor, 5 post docs, 4 doctoral students, 3 graduate students, a secretary and a technician.

Prof. Dr. Maija-Riitta Hirvonen

Prof. Hirvonen graduated in 1986 from the M.Sci program (Environmental sciences) at the University of Kuopio (now University of Eastern Finland, UEF) and in 1991 with a PhD degree in toxicology at the same university. For post doctoral studies, from 1992 to 1994, she joined Burroughs Wellcome Co., Department of Cell Biology, USA. Since 1994 she has been docent in environmental toxicology at the faculty of Natural and Environmental Sciences, University of Kuopio. In 2007 she was appointed as research professor at the Public Health Institute (now National Institute for Health and Wellfare, THL) and professor in environmental toxicology at UEF. Since January 1, 2011, she has been Vice-Dean in the Faculty of Natural Sciences and Forestry at UEF.

She is the leader of the toxicology group on air pollution in vitro and in vivo. The multidisciplinary studies of her research group are focused on mechanisms of cell death and activation of immunological defense mechanisms of adverse health effects by microbes in indoor air, urban air particulate matter and source specific emissions. The group also participates in studies on microbial exposure and development of allergy and immunological function in early life. She has 154 original peer-reviewed articles in international scientific journals and supervised 11 PhD theses on air pollutants originating from indoor air, urban air and specific combustion sources.

Dr. Pasi Jalava

Dr. Jalava graduated in 2003 from M.Sci program of Applied Zoology at the University of Kuopio. He did his Ph.D in Environmental Health for University of Kuopio and graduated in 2008. During Ph.D studies he was working in National Public Health Institute of Finland. Pasi Jalava has about 9 years experience in toxicological studies of air pollution particles. He has a strong background in different studies of air pollution, e.g. research on inflammation, cytotoxicity, genotoxicity and oxidative stress, induced by particulate matter from outdoor air, combustion sources and diesel engines. Since 2005, he has published 19 original peer reviewed articles in appreciated international journals and presented his findings in several international conferences. He has worked on several national and international research projects that have been funded by European Union Framework programmes, Tekes, and European regional development and social funds. He has also worked in Kantiva bioenergy research center of University of Eastern Finland where he has been coordi-

nating of advancement of the toxicological research related to bioenergy production and use. He is supervisor in three current PhD thesis projects at UEF. Pasi Jalava will start his post doctoral period of one year in Fraunhofer Institute for Toxicology and Experimental Medicine starting from May 2012. Jalava is working in novel multidisciplinary research line for aerosol toxicology at UEF. The air-liquid-interface systems, developed will form basis for the high quality research in the aerosol toxicology

Key Publications

Jalava PI, Salonen RO, Hytönen K, Pennanen AS, Happo MS, Markkanen P, Tissari J, Frey A, Hillamo R, Jokiniemi J, Hirvonen MR; Effect of combustion condition on cytotoxicity and inflammatory responses induced by residential wood combustion particles, Atmospheric Environment, 44(13), 1691-1698 (2010).

Happo MS, Salonen RO, Hälinen AI, Jalava PI, Pennanen AS, Dormans MA, Gerlofs-Nijland ME, Cassee FR, Kosma VM, Sillanpää M, Hillamo R, Hirvonen MR; Inflammation and tissue damage in mouse lung by single and repeated dosing of urban air coarse and fine particles collected from six European cities, Inhalation Toxicology, 22(5), 402- 416 (2010).

Jalava PI, Tapanainen M, Kuuspalo K, Markkanen A, Hakulinen P, Happo MS, Pennanen AS, Ihalainen M, Yli-Pirilä P, Makkonen U, Teinilä K, Mäki-Paakkanen J, Salonen RO, Jokiniemi J, Hirvonen MR; Toxicological effects of emission particles from fossil- and biodiesel-fueled diesel engine with and without DOC/POC catalytic converter, Inhalation Toxicology, 22, 48-58 (2010).

Web

www.uef.fi/intola

Fine Particle and Aerosol Technology Laboratory (FINE), Department of Environmental Sciences, Kuopio, Finland

Research carried out in the Fine Particle and Aerosol Technology Laboratory is focused on aerosols and high temperature processes. The main research areas and strengths are fine and nanoparticles in material synthesis and combustion. Research is carried out on fine particle issues in various combustion processes, engine emissions, nanoparticle synthesis and health&safety aspects as well as aerosol sampling, dilution and characterisation techniques. The research area covers the complete chain from fine and nanoparticle particle formation and behaviour all the way up to the sampling and dilution of particles into the ambient air and their health risks. The research is assisted by particle formation and behaviour modelling techniques, but the main work is done in the experimental research. The research equipment for real-time particle measurements and for the composition analysis of particles and organic compounds is of international top-level standard at the FINE-laboratory. In material synthesis the main focus is on gas phase synthesis of nanoparticles with atmospheric pressure chemical vapour deposition (APCVD) and physical vapour deposition (PVD) methods. With these methods extremely pure tailored functional nanocomposite materials can be produced.

In the FINE laboratory, the staff includes 21 members: a professor, 4 post docs and 12 doctoral students, a secretary, a service engineer and 2 graduate students.

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Prof. Dr. Jorma Jokiniemi

Prof. Jokiniemi received his Ph.D. in 1990 from the University of Helsinki on the topic "The effect of airborne hygroscopic matter on aerosol behaviour in severe nuclear power plant accidents" after graduating from the University of Helsinki in 1984. In 1991 his research interest moved to combustion aerosols and chemistry. In 1995 he received the status of docent from Helsinki University of Technology. In 2005 he was appointed as professor of fine particle technology at the University of Kuopio and research professor on the same topic at Technical Research Centre of Finland (VTT). From 1991 to 2005 he was the head of the research group "Aerosol Technology" at VTT, and since 2005 he has been the Director of the "Fine Particle and Aerosol Technology Laboratory – FINE" at the University of Eastern Finland. Prof. Jokiniemi has over 28 years experience in fine particle and aerosol research. He has supervised eight doctoral theses, 109 peer-refereed papers, more than 500 other publications and nine patents.

Key Publications

Kaivosoja T, Viren A, Tissari J, Ruuskanen J, Tarhanen J, Sippula O, Jokiniemi J; Effects of a catalytic converter on PCDD/F, chlorophenol and PAH emissions in residential wood combustion, Chemosphere, in press (2012).

Ruusunen J, Tapanainen M, Sippula O, Jalava PI, Lamberg H, Nuutinen K, Tissari J, Ihalainen M, Kuuspalo K, Mäki-Paakkanen J, Hakulinen P, Pennanen A, Teinilä K, Makkonen U, Salonen RO, Hillamo R, Hirvonen MR , Jokiniemi J; A novel particle sampling system for physico-chemical and toxicological characterization of emissions, Analytical and Bioanalytical Chemistry, 401(10) 3183-3195 (2011).

Jokiniemi J, Lazaridis M, Lehtinen K, Kauppinen E; Numerical simulation of vapour-aerosol dynamics in combustion processes, Journal of Aerosol Science, 25(3), 429 - 446 (1994).

Olli Sippula, Ph.D.

Olli Sippula received a Master's degree on Environmental Engineering at the University of Oulu in 2004 and a PhD degree on Environmental Science at the University of Eastern Finland in 2010 with a thesis titled "Fine particle formation and emissions in biomass combustion". He has nine years of experience in studies related to combustion aerosols, emission reduction technologies, fine particle sampling methods and ash behaviour and chemistry in biomass combustion. He has worked as a development manager in the Kantiva bioenergy research center of UEF and as project manager in a number of research projects. He is currently a supervisor of four Ph.D. theses and has about 70 publications of which 14 are original peer reviewed articles. He will start a one year post-doctoral period at the University of Rostock in the Joint Mass Spectrometry Centre in June 2012.

Key Publications

Sippula O, Hokkinen J, Puustinen H, YliPirilä P, Jokiniemi J; Comparison of particle emissions from small heavy fuel oil and wood fired boilers, Atmospheric Environment 43, 4855-4864 (2009).

Sippula O, Lind T, Jokiniemi J; Effects of chlorine and sulphur on particle formation in wood combustion performed in a laboratory scale reactor, Fuel 87(12), 2425-2436 (2008).

Sippula O, Hytönen K, Tissari J, Raunemaa T, Jokiniemi J; Effect of Wood Fuel on the Emissions from a Top-Feed Pellet Stove, Energy & Fuels, 21(2), 1151- 1160 (2007).

Web

www.uef.fi/fine

University of Cardiff

THE CARDIFF SCHOOL OF BIOSCIENCES IS BEST KNOWN FOR THE WORK OF ITS FORMER DIRECTOR, PROFESSOR SIR MARTIN EVANS FRS.

This work was recognized by Sir Martin's Nobel Prize in Physiology or Medicine 2007 (together with Mario Cappechi and Oliver Smithies) "for their discoveries of principles for introducing specific gene modifications in mice by the use of embryonic stem cells". Under its current director, Medical Research Council Professor Ole Petersen CBE FRS, who pioneered patch clamp single channel recordings in epithelial cells and discovered intracellular calcium tunnels in exocrine gland cells, the School provides a dynamic and stimulating research environment with impressive modern facilities and high-calibre research-active staff. The Cardiff School of Biosciences is one of the largest bioscience departments in the UK. Supported by state-of-the-art facilities, its topical courses and cutting-edge research spans the full range of the Life Sciences from whole (eco) systems to molecular biology.

Dr. Kelly BéruBé

She is the Director of the Lung & Particle Research Group at the School of Biosciences, Cardiff University, UK. With a background in electron microscopy and lung toxicology, she has built an international reputation in the field air pollution and human health and holds numerous appointments in the USA and UK on funding bodies, advisory councils, professional societies and journal editorial boards that focus on environmental health. Her research focuses on the determination of intelligent biomarkers of exposure and harm in the respiratory system, with a particular interest in understanding how pollutants compromise lung biochemistry and alter gene and protein expression to drive disease mechanisms.

Dr. BéruBé's research has been recognised with a number of awards, including the Institute for Science & Health (USA) "Scientific Merit Award 2006" for toxicogenomics of inhaled xenobiotics and the honour of being the British Toxicology Society "Australasia Visitor 2006" to conduct a coast-to-coast lecture tour on nano-toxicology. Current work on "human tissue equivalents of respiratory epithelia", as viable in vitro alternatives for in vivo inhalation toxicology, was awarded the UK NC3Rs "Replacement Prize" and the "Science & Technology Innovation Prizes" in 2007 and 2010. Dr BéruBé's field of study is of natural interest to the general public, and as such, she is a prolific science writer and popular invited speaker, and has worked extensively on communicating her research through public engagements of science for primary schools, laymen groups and professional learned societies.

Dr. Tim Jones

- Director of Taught Postgraduate Programmes
- Head of Applied Environmental Geoscience Research Group
- Joint leader of the Particle and Lung Research Group
- Deputy directory, M.Sc. Applied Environmental Geology
- Admissions Officer MSc

Academia

- PhD RHBNC (University of London) 1991
- 2005-present: Senior lecturer in Applied Environmental Geology, Earth Sciences, Cardiff University
- 2001-2005: Lecturer in Applied Environmental Geology, Earth Sciences, Cardiff University
- 1998-2001: Senior Research Associate, School of Biosciences, Cardiff University
- 1995-1997: University Research Fellow, Dept. Earth Sciences, Cardiff University
- 1992-1995: Assistant Professor and Humboldt Fellow, Institut und Museum fuer Geologie und Palaeontologie, Eberhard-Karls-Universitaet Tuebingen, Germany
- 1991-1992: Post-doctoral researcher, Royal Holloway and Bedford New College, University of London

Research

Dr. Tim Jones is co-leader of the interdisciplinary Particles and Lung Research Group (PLRG) with Dr. Kelly BéruBé in Biosciences, Cardiff. The PLRG won the IFSH Dietrich Hoffman Scientific Merit Award in 2006, and the NC3Rs Replacement prize 2007.

Ailsa Langford

Is a recent graduate from the School of Biosciences, Cardiff University, Wales, UK. She graduated with a BSc (1st class, honours) degree in Biomedical Science. Her PhD project will involve the „determination of the oxdicative capacity of air pollution from different European Union pollution zones". This project will be supervised by Dr Kelly BeruBe and Dr Tim Jones (Cardiff University, UK) and Professor Ralf Zimmerman (Rostock University, DL).

From top left to bottom right: Tim Jones, Kelly BéruBé and Ailsa Langford.

Key Publications

BéruBé KA, Jones TP, Housley GH, Richards RJ; The Respiratory Toxicity of Airborne Volcanic Ash from the Soufriere Hills Volcano, Montserrat, Mineralogical Magazine, 68(1), 47-60 (2004).

Dr T. Jones (PI) and Prof. C. Harris (EARTH), Dr K. BeruBe (BIOSCI).

Jones TP, Williamson BJ, BéruBé KA, Richards RJ; Microscopy and chemistry of particles collected on TEOM filters: Swansea, south Wales, 1998-1999, Atmospheric Environment, 35(21), 3573-3583(2001).

Web

www.cardiff.ac.uk/biosi

HICE › Aerosols and Health
Helmholtz Virtual Institute of Complex Molecular Systems in Environmental Health

ASG Analytik-Service Gesellschaft

ASG IS AN INDEPENDENT, PRIVATELY OWNED SERVICE PROVIDER.

Fields of activity include analytical laboratory for solid, liquid and gaseous fuels, consulting services, process optimisation, production of QC materials and test fuels, and manufacture of instruments for fuel analysis and emissions.

As the first European laboratory with an ISO 17025 accreditation for biofuels, we primarily specialise in answering all analytical and technical questions concerning biodiesel, bioethanol and vegetable oil fuels. Our analytical service comprises testing of all parameters according to national and international specifications (EN 14214, ASTM D 6751, DIN 51605, etc.).

Furthermore, we proudly present our new ASG Customer Center for Biodiesel Process Development. Here you can carry out the whole process chain yourself: From the raw material to the end product. You can work with the optimum procedures enabled by our fully up-to-date mini-plant laboratory.

Dr. Thomas Wilharm

Dr. Wilharm is general manager of ASG Analytik-Service Gesellschaft.

His professional experience includes:

- Work experience in the field of biofuels since 1993.
- Member of CEN working group 632.1, biodiesel specification.
- Member of CEN TC 307 JWG Validation of EN 14214.
- Quality auditor for the German biodiesel industry and the international BIPAC program of AGQM.
- Member of the European „Bioscopes“ project: Development of biodiesel testing methods.
- Different projects: Process improvement for the biodiesel industry.
- Training courses in analytical skills for lab staff and engineers in the petrochemical and biodiesel industry.

Web

www.asg-analytik.de

VITROCELL® Systems GmbH

VITROCELL® SYSTEMS HAS OVER 10 YEARS OF EXPERIENCE IN THE DEVELOPMENT, PRODUCTION, INSTALLATION, AND TRAINING FOR ADVANCED EQUIPMENT FOR IN VITRO STUDIES.

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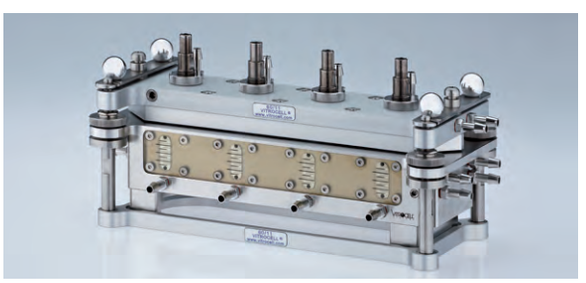
Contribution to HICE

Design and delivery of cell culture exposure systems.



VITROCELL® Cultivation and Exposure Systems: The systems are used for the exposure of aerosols to lung cells at the air/liquid interface. The company produces a broad range of modules for cell culture inserts in 6-well, 12-well and 24-well sizes. The customer receives complete solutions for the smaller lab as well as for higher throughput.

Tobias Krebs

Tobias Krebs was born in 1956; Managing Partner and Founder; Industrial Engineer, Munich Polytechnic and MBA, INSEAD.

Web

www.vitrocell.com

Decodon GmbH

DECODON GMBH IS A BIOINFORMATICS COMPANY THAT DEVELOPS INNOVATIVE SOFTWARE FOR THE MODERN LIFE SCIENCES.

DECODON GmbH is a bioinformatics company that develops innovative software for the modern Life Sciences. Its bioinformatics tools are helping scientists to generate knowledge from the massive amounts of data that are accumulated by recent methods in global functional genomics.

The company brings together specialists with diverse backgrounds from Molecular Biology, Computer Science and Mathematics. Software development at DECODON is driven by the needs of leading researchers in the field of functional genomics and realised by using advanced methods from various areas of Mathematics and Informatics. DECODON's products prove the efficiency of this approach.

The company has its offices in Greifswald, in direct neighborhood to biotech companies as well as the institutes of Micro and Molecular Biology, and Mathematics and Computer Science at the University of Greifswald. Close cooperation with these and other academic institutions gives DECODON access to state of the art technology and methods in both Life Sciences and Informatics. Cooperations exist with companies providing complementary products.

DECODON is a well-positioned niche company with cutting-edge technology, a professional development team and highly qualified management. DECODON is well known in the academic and industrial proteomics markets and wants to further penetrate those markets.

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Photonion GmbH

PHOTONION IS AN INNOVATIVE COMPANY DEDICATED TO PROVIDING CUSTOMISED SOLUTIONS FOR MONITORING CHEMICAL COMPOUNDS.

Photonion GmbH was founded in 2009 as a spin-off from Helmholtz Zentrum München.

The goal of Photonion is to develop and distribute new analytical devices based on mass spectrometric methods in order to analyse complex organic gases, liquids or solid materials. Potential applications include process control at combustion, pyrolysis or roasting plants. The analysis of cigarette smoke, of polymers, or crude oil are further applications. Soft ionisation methods, in particular the ionisation with UV light is preferred.

The actual technology is based on one-photon ionisation, based on an innovative vacuum ultraviolet light source. The advantage of this ionisation method is that substances can be measured directly in complex mixtures. Time-consuming separation techniques combined with MS (e.g. GC) are not needed. This is why MS containing soft ionisation is ideally suited for process monitoring and quality control applications.

The headquarters of Photonion are located in Schwerin (Hagenower Str. 73, 19061 Schwerin, Germany) and the research and development division are located in Munich (Helmholtz Zentrum München, building 38c, Ingolstädter Landstr. 1, 85764 Neuherberg, Germany).

General managers are Wolf Münchmeyer and Dr. Andreas Walte. Both are also founders and general managers of the company Airsense Analytics GmbH.

Wolf Münchmeyer

Dr. Andreas Walte

Web

www.photonion.de

JRC and Sustainable Transport Unit (STU) – VELA Laboratory

THE JOINT RESEARCH CENTRE IS THE SCIENTIFIC AND TECHNICAL ARM OF THE EUROPEAN COMMISSION.

The mission of the JRC is to provide scientific advice and technical know-how to support a wide range of EU policies. Its status as a Commission service, which guarantees independence from private or national interests, is crucial for pursuing its mission.

The JRC has seven scientific institutes, located at five different sites in Belgium, Germany, Italy, the Netherlands and Spain, with a wide range of laboratories and unique research facilities. Through numerous collaborations, access to facilities is granted to scientists from partner organizations.

Many of the complex challenges ahead cut across traditional policy boundaries and require multi-disciplinary research. In order to deliver the best support, the JRC focuses its efforts on seven thematic areas, which respond to major EU and global challenges and take into account the JRC's proven competences.

One of the seven institutes of the JRC is the Institute for Energy and Transport. Inside this structure and since early 2000 the Sustainable Transport Unit (formerly Transport and Air Quality Unit) has been supporting the development and implementation of the future European emissions standards through research strongly based on experimental activities conducted in its Vehicle Emissions Laboratory (VELA).

The VELA laboratory is one of the very few laboratories in Europe where all kinds of vehicles can be tested for complete emission characterization.

Several projects supporting key EU emission policies have been carried out and completed in the recent years. A visible example is the validation of the methodology to measure particle number of particles emitted by diesel vehicles and the related emission limit which is now part of the current Euro 5 emission standards.

More recently the attention was focused on the emissions from modern and new vehicle concepts under laboratory and real world driving conditions with conventional and alternative fuels.

Moreover, the emission data collected have allowed updating the emission factors of regulated and unregulated pollutants of contemporary engine/vehicle technologies running on conventional and alternative fuels (gaseous fuels and biofuels). This activity is of great important to estimate the contribution of traffic to air pollution which is still a big problem in many European urban areas.

Dr. Maria C. Astorga Llorens

She is Senior scientific officer and project leader at JRC-Sustainable transport Unit. She is in charge of the development and implementation of the analytical techniques to characterize unregulated pollutants emitted by vehicles. She has followed the application of innovative techniques, like the use of FT-IR instruments to monitor on-line specific compounds in the exhaust emissions. From 2010, she has been co-chairing the United Nations working group in charge of identifying currently unregulated pollutants which will be included in future worldwide harmonized test procedure for light duty vehicles.

Thematic Areas

- Towards an open and competitive economy
- Development of a low carbon society
- Sustainable management of natural resources
- Safety of food and consumer products
- Nuclear safety and security
- Security and crisis management
- Reference materials and measurements

VELA experimental facility for Light Duty vehicles and mobile smog chamber from PSI during 2011 campaign in Ispra (Italy).

Web

iet.jrc.ec.europa.eu

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