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CITE RESEARCH INITIATIVE

# Chemicals in the Environment (CITE)

## Report of the First Annual Conference of the Helmholtz research topic CITE

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In 2009, the two Helmholtz research centres, Forschungszentrum Jülich and UFZ Helmholtz Centre for Environmental Research, Leipzig, started the novel research topic CITE (Chemicals in the Environment). CITE involves the collaboration of around 100 scientists to address major questions on the fate, effects and management of chemicals in the environment. Modern societies develop, produce and use chemicals in large numbers and quantities for purposes covering many applications such as cleaning, painting, process manipulation or pharmaceutical treatment. At the same time, the current means of assessment of chemicals' behaviour in the environment have proven to neither be able to cover the sheer number of commercially available compounds, nor has chemical management been able to avoid severe incidences of unintended chemical environmental occurrence or adverse biological effects.

Therefore, a joint effort seemed to be timely to meet societal demands for improved prospective assessment as formulated in EU settings such as the REACH[1] regulation, the directives for Biocides, Pesticides, Pharmaceuticals, or the Water Framework Directive for environmental quality standards. Within the CITE research initiative, we intend to provide novel routes to the assessment and management of chemicals' fate and effects from a process perspective and on a mechanistic basis. This will be done in collaboration with academic, industrial and regulatory partners at the national, European and international level. We have geared our activities towards research on

- chemodynamics,
- accumulation and transformation of chemicals in soil,
- ecology of biodegradation, and
- biological effects of contaminants.

[1] *R*egistration, *E*valuation, *A*uthorisation and Restriction of *Ch*emicals.

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Moreover, as we intend to utilise our enhanced understanding to improve the process control of chemical mass transfer, we additionally consider environmental technologies and provide technology demonstration platforms. Furthermore, several topics including transport processes and modelling, interface processes and the role of biofilms as well as nano-particles span the cluster topics. The first year of research activities resulted in more than 100 ISI-cited publications on the various issues identified as being of major importance. These were presented and discussed at the First Annual Conference of the CITE consortium in Leipzig, 23 March 2010. Subsequently, a brief summary of the nine sessions is provided.

Amongst the huge number of chemicals of environmental concern, so far only a limited number have been characterised with respect to their environmental behaviour. In the session *Chemodynamics*, efficient and reliable tools for the evaluation of their environmental fate were discussed, specifically focussing on the environmental fate of structurally difficult organic compounds, environmental processes, and fate of elements and their species.

The nine platform lectures presented the issues

- modelling of transfer processes, chemical fate (sorption, bioaccumulation, degradation) and structure–activity relationships,
- analytical methods to study the transfer processes and metabolisation of polar organic, especially bioaccumulating substances, pharmaceuticals and organometalloid compounds,
- procedures for dynamic fractionation and coupled chemical and ecotoxicological assessment of arsenic species.

These topics and additional contributions on nano-particles, isotopes as tracers for contaminant behaviour and validation of analytical methods were covered through 19 additional posters.

The session *Transformation in Soil* covered three main topics. The first topic dealt with microbial aspects of degradation and biodegradation of xenobiotics. *Anja Miltner* reported on the use of labelled xenobiotic carbon by soil microorganisms as an energy source and its inclusion into microbial cell material (fatty acids, proteins). This integration of carbon from labelled xenobiotics often leads to an overestimation of bound xenobiotic residues because fragments originating from microbial cell wall envelopes bind to mineral particles. *Nicolai Jablonowski* reported on the influence of biochar and activated carbon on the biodegradation of atrazine. In atrazine-adapted soils, biochar revealed a stimulating effect while activated carbon inhibited the atrazine degradation.

The second topic encompassed the sorption and transformation of xenobiotics. *Jing Zhang* was able to distinguish between partitioning of pyrene to amorphous organic carbon (AOC) and adsorption on black carbon (BC) as the main interaction types in Yangtze river sediments and emphasised the importance of BC in pyrene immobilisation under environmental conditions. *Stephan Sittig* and *Roy Kasteel* reported on the long-term and short-term sorption and transformation of sulfadiazine (SDZ). The long-term study focussed on the extraction and determination of SDZ transformation products. Besides known metabolites, four yet unidentified metabolites were found. The short-term study presented a combined kinetic and sorption model (two stages – one rate, 2S1R) to describe non-equilibrium sorption and transformation of SDZ in soils.

Finally, the last topic, presented by *Hans Lewandowski*, dealt with quantum chemical calculations of NMR shifts to elucidate the structure of bound 2-aminobenzothiazole (ABT) residues. Comparison between experimental and calculated NMR shifts revealed proton transfer in ABT adducts with 3-aminobenzoic acid and thiophene-2-carboxylic acid.

The session *Ecology of Contaminant Biodegradation* presented research on the role of microbial communities as key drivers of the vital ecosystem service of transformation of contaminants in natural and constructed environments. Most of the research was inspired by the questions of "who is where and why in microbial ecosystems", and how humans can make use of this mechanism-based knowledge for targeted contaminant removal.

Several papers addressed the question of microbial diversity and its relation to ecosystem functioning and its reactions to change and disturbance regimes, respectively. Various contributions demonstrated the relevance of both bacterial and protistan predator richness for compound turnover, the impact of plant-litter-derived hydrocarbons on microbial communities or syntrophic interactions in anaerobic benzene degradation. The session's papers included experimental approaches covering a continuum of environmental complexities from simple, constructed communities in fully controlled laboratory environments to real contaminated sites. Systems studied included high-throughput laboratory systems, constructed wetlands at UFZ's SAFIRA II research facility or BTEX and MTBE-contaminated aquifers. Other highlights focused on the analyses of in situ microbial communities at differing biogeochemical interfaces by state-of-the-art microscopy and molecular biological techniques as well as structure–function relationships by novel stable isotope-based proteomic approaches, respectively.

The exciting session, in summary, made obvious that research into complex and highly adaptive microbial communities requires a combination of experimental research into the autecology and community ecology of degraders, observation of real contaminated ecosystems and ecological modelling.

The CITE research cluster *Biological Effects of Contaminants* focuses on the diagnosis and prediction of the effects of individual chemicals and complex mixtures on biological

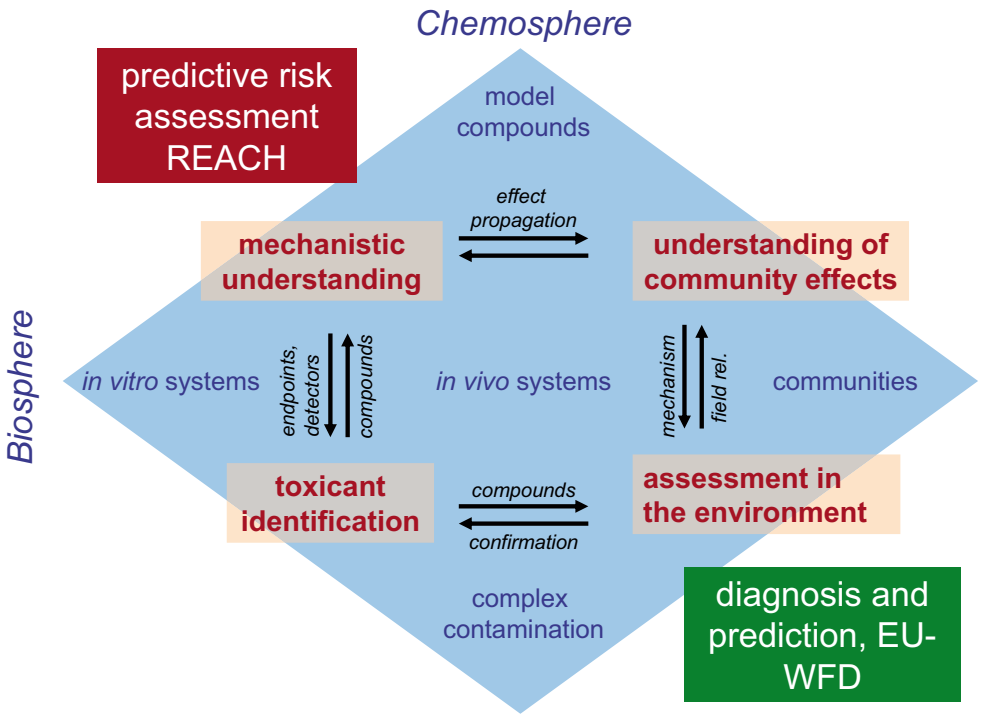


**Fig. 1** Focal points of the biological effect research

systems and thus represents a major link between the biosphere and chemosphere. There is a close link with societal needs with a focus on 1) predictive risk assessment of individual toxicants to meet the requirements of REACH and 2) on diagnosis and prediction of effects of complex mixtures of chemicals on ecosystems related to the EU Water Framework Directive.

The interdisciplinary effect cluster is organised around the four closely interlinked focal points 1) mechanistic understanding of effects on a molecular, cellular and organism level, 2) understanding of community effects, 3) assessment of effects in the environment, and 4) toxicant identification (Fig. 1).

Presentations and posters demonstrated significant progress in all four areas. Starting with the assessment of chemicals in the environment, novel integrated monitoring strategies were presented. The concept of pollution-induced community tolerance (PICT) was shown to be a powerful tool to understand and assess toxic effects at the community level. The interaction of different stressors was demonstrated for the mutual influence of antibiotic and heavy-metal resistance of microbial communities. A presentation on sediment assessment and a question on the relevant toxicants opened a discussion on tools for the identification of causative toxicants in complex environmental contaminations as well as the role of bioavailability. Using the transformation products of diclofenac as an example, effect-directed analysis (EDA) was presented as a tool to identify toxic components of a mixture. A new challenge for EDA is the identification of polar, multifunctional toxicants in complex mixtures, which is approached with novel analytical techniques (LC-LTQ Orbitrap) and powerful computer tools. Mechanistic understanding of exposure and effects was highlighted as a crucial precondition to approach societal needs to assess a multitude of chemicals in the context of REACH avoiding excess animal testing, which is costly and ethically more than questionable. Surrogates such as embryo tests and novel mechanism-based tools including toxicogenomics, the assessment of active cellular transport mechanisms and mechanistic effect models are major tools in the CITE toolbox to solve this problem.

Important challenges for the effect cluster in the future were identified including toxicity prediction for compounds with reactive and specific modes of action including a better understanding of exposure, the focus on polar and ionic compounds with respect to sorption, uptake in organism, isolation from complex mixtures and identification, the combination of PICT-based approaches with "omics" techniques for a better understanding of community effects, and integrated trait-based approaches for the assessment of toxic stress in multiple stressed environments involving stressor-specific metrics, ecological understanding and modelling.

The first part of the session *Process Control and Environmental Technologies* was devoted to physical and chemical technologies for contaminants' removal from soil, water and off-gas flows. Radiofrequency-induced heating, originally developed for soil remediation has recently been adapted to gas treatment by means of "thermochromatographic pulses"

allowing the combination of adsorption, catalysis and desorption in a single gas-treatment reactor. For water treatment, both reduction and oxidation processes are important, depending on the type of pollutant present. Reduction of halogenated hydrocarbons may be promoted by Carbo-Iron, whereas advanced oxidation processes may allow efficient oxidation of most organic pollutants in groundwater and wastewater.

The second part of the session was devoted to *Biotechnology*. For the treatment of polluted wastewater, constructed wetlands may play an important role, and a thorough understanding of the processes involved is the prerequisite to control and enhance pollutants' removal by these systems. Examples presented included the dynamics of sulphur compounds in constructed wetlands and the effect of oxygen availability on the expression of genes related to anaerobic and aerobic degradation of toluene. Finally, the biotechnological production of a chiral alcohol by a novel monooxygenase from an MTBH-degrading bacterium was presented. This final presentation again provided an example of the possibility to adapt technologies developed for a given problem (MTBH degradation) to another goal (environmentally friendly production of a chemical).

The current main focus of CITE activities to provide a *Technology Demonstration Platform* is the application and further development of novel soil and groundwater investigation and remediation technologies as well as their demonstration within contaminated land management strategies. Most of the remediation technologies being tested at the well equipped field sites were presented in the other sessions. The presented topics of this session included novel monitoring techniques as well as management tools for contaminated land.

The technical applications covered indoor measurements to monitor the influence of contaminated groundwater and soil on indoor air, and as a second example the application of geo-electric techniques for a fast and non-invasive screening for acid mine drainage zones. The second part was dominated by discussion of a novel tool for the management of mega-sites – the SAFIRA II Management System – and the value assessment of contaminated land. Another major issue of the cluster includes TASK activities for improving market accessibility of emerging knowledge and new technologies. These activities were demonstrated by one example – the MAGPROX, a monitoring tool for metal contamination using magnetic proxies.

The session *Transport Processes and Modelling* consisted of four talks, with one talk reporting on field applications employing environmental tracers, and three talks focusing on reactive transport modelling efforts in more theoretical settings. The modelling approaches presented span the whole range of spatial scales relevant to reactive transport problems. All models consider the degradation of a contaminant by microorganisms colonising the soil matrix. For the micro-scale, *Martin Thullner* presented a mathematical framework to describe transport and biodegradation in an idealised single pore. The model allowed studying the relation between mass transfer processes, bioavailability and biodegradation. *Mehdi Gharasoo* connected single pores to form a transport network. The focus of his reactive transport simulations of such pore networks was on the influence of spatial heterogeneities on bioavailability and degradation activity at the meso-scale. *Florian Centler* presented a flexible reactive transport simulator for addressing reactive transport problems at the macro-scale. The simultaneous fractionation of the stable isotopes of carbon and hydrogen during microbial degradation following two alternate pathways was considered in a simulation study, and the significance of this 2D isotope analysis for the identification and spatial localisation of the active pathway was discussed. Stable isotopes were also used by *Michael Schubert* in several field applications. He reported on the use of environmental tracers, including stable isotopes and radio isotopes, at several field sites to identify the origin of contaminated water and its residence time in the subsurface, as well as the sources of heavy metal contaminations.

In the session on *Interfaces/Biofilms* four talks were presented, two of them focusing on processes at the mineral surface and two addressing the impact of fungal hyphae on the translocation of contaminants and bacteria in soils. For the analysis of the metabolic activity of biofilms, *Thomas Maskow* presented a miniaturised chip-calorimetry, which was used to study the response of biofilms to different toxic agents. *Frauke Schnitzler* introduced a method for calculating the distribution of organic carbon and xenobiotics between clay and silt/sand fractions of soils using BET-N2 measurements. The importance of fungal networks for the accessibility of bacteria to soil contaminants was shown experimentally in the presentation by *Lukas Wick*. Some of these results were the basis for the theoretical study presented by *Thomas Banitz*, where numerical simulations were used to quantify biodegradation rate improvements by different fungal network architectures. In combination, these talks highlighted the broad range of processes affecting the fate of chemicals in soil systems.

The session on *Nano-particles* comprised three oral presentations. The interest of the audience was immense, which was not only expressed by the number of listeners but also by the lively discussion. All three presentations were connected to the application of the materials itself, particle synthesis, or the use of tools emitting the particles. This also reflects the importance of the nano-particle utilisation and application-related occurrence of nano-particles and nano-structures. We learned that nano-particles bear a high potential for uses in environmental clean-up processes such as

water purification. The audience also showed a great interest in the applications themselves.

The session showed that accompanying ecotoxicological studies of the environmental effects of the particles are very important in order to guarantee their sustainable use in open applications. So far, cell toxicological tests have been conducted. In the future further test assays on biologically more complex system levels will be carried out. The interdisciplinary work between technologically oriented approaches and ecotoxicological studies is well appreciated.

A new nano-sized material should be treated as a new chemical including the demanded awareness of all the issues and concerns surrounding it. A full characterisation of the nano-particles and of their behaviour is necessary in order to minimise risks accompanied with their utilisation. In ecotoxicological studies the effects of single particles, agglomerates, and those derived from solutes should be well differentiated. We also learned in the session that all the investigated particles were able to enter living cells, and although only some showed obvious effects on cell vitality, their overall biological potencies remains to be described. The field is still new and there is a lot more to learn about nano-particles, their impacts on the environment and humans and their safe utilisation in environmental applications.