Reorientation of the Department of Ecological Chemistry (OEC) at the Helmholtz-Centre for Environmental Research – UFZ in Leipzig



Graphical abstract

With the retirement of the long-standing appreciated Head of Department, Prof. Gerrit Schüürmann, the Department of Ecological Chemistry at the Helmholtz-Centre for Environmental Research - UFZ was taken over by the environmental chemist Prof. Annika Jahnke on Oktober 1, 2022. She returned to Germany in 2014 following 7 years at Stockholm University, to build up a research group at UFZ. Next to the research at UFZ, amongst others in third-party funded projects supported by the European Research Council ERC, the BMBF and the Helmholtz Association of German Research Centres, Annika Jahnke took over a joint professorship in "Exposome Analytics" together with RWTH Aachen University in June, 2020. As part of the professorship at the Department of Biology within Faculty 1 for Mathematics, Computer Science, and Natural Sciences she teaches mainly in the BSc and MSc programs of Biology and Ecotoxicology.

Orientation and Research Topics

In the framework of the transfer of the department (graphical abstract) we channeled our research efforts to an overall key goal, i.e., to characterize the environmental behavior of relevant organic chemicals, including those that are associated with microplastics.

The behavior of chemicals in the environment is governed by their source of emission, their reactivity, their physicochemical properties (solubility, sorption, volatility, ...), and the gradient in chemical activity between different environmental media. Moreover, core factors including partitioning, degradation, bioaccumulation, and biotransformation have a large impact on the environmental behavior of chemicals. To characterize the fate of relevant organic chemicals in the environment, we develop specific approaches for their analytical determination, including suitable experimental design and specific target analysis as well as models to predict their behavior in abiotic environmental compartments and organisms.



Figure 1. Colleagues at the Department of Ecological Chemistry in November, 2022 (Picture: Klaus Seyfahrt, UFZ).

The research activities of the Department of Ecological Chemistry focus on the following areas:

(i) An important research topic of the department is the enrichment of diverse environmental chemicals in biota including top predators. We develop innovative passive samplers to study chemicals from abiotic and biotic media. Amongst the passive sampler formats that we use are passive equilibrium sampling devices, so-called "chemometers" (www.ufz.de/chemo-risk, mostly based on the polymer silicone), that, after equilibrating with different media, ensure direct comparability of the chemical concentrations in the chemometers across media and thus allow for conclusions about the chemicals' environmental fate (Rojo-Nieto & Jahnke 2023). Using such chemometers, we investigate amongst others abiotic media like sediment (Muz et al. 2020), aquatic organisms along trophic webs (e.g. mussels, non-predatory and predatory fish, Rojo-Nieto et al. 2019, Wernicke et al. 2022), and different tissues of marine mammals (Reiter et al. 2023).

Following this approach, which allows to study the ratio of chemical activity between environmental compartments or different biota species as the driver for bioaccumulation, and together with diverse partner institutions, we investigate the exposure of environmental organisms (amongst others marine and terrestrial mammals) and in the future also humans towards mixtures of environmental chemicals (www.ufz.de/exposo-meter). Within our work with biota we determine the totality of chemical exposure of diverse species over their entire lifecycle, including exogenous and endogenous chemicals as well as degradation products that taken together constitute the so-called "exposome" of the studied individual (contacts: <u>annika.jahnke@ufz.de</u> & elisa.rojo-nieto@ufz.de).

(ii) In addition to the exposure towards chemicals we also study their reactivity. In the environment, our primary focus is on hydrolysis because it has a big impact on the fate and bioavailability of chemicals. Moreover, reactivity of chemicals towards proteins is the key for the development of skin and respiratory allergies. To characterize reactivity, we develop socalled "chemoassays" (Böhme et al. 2016, 2021) which allow retrieval of toxicologically relevant information on reactivity and hence facilitate, amongst others, predictions of the allergenic potential of chemicals, representing an alternative to traditional animal testing. In addition to our chemoassay studies, we focus on the metabolism of the amino acid tryptophan: Together with colleagues from the German Cancer Research Centre we have established a method to specifically quantify tryptophan metabolites (Sadik et al. 2020) (contact: alexander.boehme@ufz.de).

(iii) Another focus is the investigation of environmental chemicals in abiotic natural and anthropogenic media including plastics. For several years, we have done research on the impact of environmental weathering of plastics on their fate and potential effects. Furthermore, we investigate the occurrence, transport and fate of plastics at hotspots and in background areas of the North Pacific Ocean (www.ufz.de/micro-fate) as well as the impact of plastics on ecosystem services and human and environmental health (www.ufz.de/p-leach). One core part are considerations regarding plastics in the environment within the planetary boundary concept (Arp et al. 2021, MacLeod et al. 2021) (contacts: annika.jahnke@ufz.de & elisa.rojo-nieto@ufz.de).

(iv) An important core of our work is the detailed description and prediction of the physicochemical properties of chemicals, which is the basis of most other activities and which is mirrored in all our projects. In our department, we both determine these properties in partitioning experiments (Ulrich & Böhme 2022) and reactivity determination (Böhme et al. 2021) but also theoretically, using different modeling approaches such as LSERD (<u>www.ufz.de/lserd</u>), deep learning (Ebert & Ulrich 2022) or as implemented in the ChemProp software (<u>www.ufz.de/</u> <u>ecochem/chemprop</u>, Ebert et al. 2023)

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(v) Last but not least, we pay particular attention to outreach activities of the Department of Ecological Chemistry. Our related work includes target-oriented science communication of our research outcomes towards expert committees and the general public. This effort has been acknowledged with the UFZ Communication Award in 2022. Amongst others, we have, together with colleagues, developed a research comic regarding the topic of plastics in the environment for the target group of daycares and elementary schools (JPI Oceans WEATHER-MIC, Figure 2) (contact: annika.jahnke@ufz.de).

WEATHER-MIC Time for Change - How it all started...



Figure 2. Research comic summarizing selected research out-comes of the JPI Oceans project WEATHER-MIC (Annika Jahnke & Dana Kühnel, UFZ).

Cited Literature:

Arp et al. *Environ. Sci. Technol.* **2021** <u>https://doi.org/10.1021/acs.est.1c01512</u> Böhme et al. *Chem. Res. Toxicol.* **2016** <u>https://doi.org/10.1021/acs.chemrestox.5b00398</u> Böhme et al. Chem. Res. Toxicol. 2021 https://doi.org/10.1021/acs.chemrestox.1c00266 Ebert & Ulrich Fluid Phase Equilib. 2022 https://doi.org/10.1016/j.fluid.2021.113349 Ebert et al. Environ. Sci. Technol. 2023 https://doi.org/10.1021/acs.est.2c05623 MacLeod et al. Science 2021 https://doi.org/10.1126/science.abg5433 Muz et al. Environ. Sci. Technol. 2020 https://doi.org/10.1021/acs.est.0c05537 Reiter et al. Environ. Sci: Processes Impacts 2023 https://doi.org/10.1039/d3em00033h Rojo-Nieto et al. Chemosphere 2019 https://doi.org/10.1016/j.chemosphere.2018.12.134 Rojo-Nieto & Jahnke ChemComm 2023 https://doi.org/10.1039/D2CC06882F Sadik et al. Cell 2020 https://doi.org/10.1016/j.cell.2020.07.038 Ulrich & Böhme Environ. Adv. 2022 doi.org/10.1016/j.envadv.2022.100284 Wernicke et al. Environ. Sci. Europe 2022 doi.org/10.1186/s12302-022-00644-w

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