

Advances in Exposure Modelling: Bridging the gap between research and application

Todd Gouin, Antonio Di Guardo

May 11, 11:05 - 12:45, Meeting Studio 313 & 315

Assessing environmental exposure of chemicals is a challenging, but critical part of performing an environmental risk assessment. Approaches to assess exposure include the use of monitoring data, often coupled with models, for chemicals that are in current use, or for chemicals not yet on the market, there is a heavy reliance on the use of exposure models to derive predicted environmental concentrations (PEC). There are various exposure models that can be utilized, and methods for deriving PECs can vary between regulatory bodies. For instance, in Europe differences in estimating PECs vary between general chemicals, regulated under REACH, plant protection products (PPP), as defined by the PPP regulation ((EC) No 1107/2009), and pharmaceuticals, regulated by the European Medicines Agency. Ultimately, it is important to ensure that exposure assessment is conducted in a manner that is transparent, robust, and takes into consideration the latest advances in scientific developments, while at the same time provides a reasonable level of conservatism, necessary to account for associated uncertainties and natural variance in the environment that might influence the reliability of PEC estimates. In this session, advances in exposure models that help to better quantify uncertainties associated with variance in environmental properties and emission scenarios used to strengthen confidence in PEC estimates are encouraged. A particular area of interest would be studies aimed at exploring opportunities for the development of harmonized approaches for assessing exposure between the different industry sector groups, and which build on the strengths of the various approaches. To this end, studies aimed at novel methods used towards improving estimates of emissions, developments in the handling of polar, ionized, and other chemicals with properties outside the applicability domain of existing exposure models, advances in tools aimed at integrating environmental fate models with ecological and/or effects models, either as screening-level or high-tiered tools are especially welcome.

Advances in the Environmental Fate of Down-the-Drain Chemicals, including Pharmaceuticals

Lisa Ann Constantine, Duane Huggett, Ed Schaefer, Jens Schönfeld

May 8, 11:05 - 12:45, Meeting Studio 314 & 316

There is an increased interest in understanding the environmental risk of Down-the-Drain (DtD) chemicals, such as pharmaceuticals and personal care products. Inherent in the environmental risk assessment (ERA) process is the conduct of environmental fate studies, such that a detailed understanding of the compartments of interest, rate kinetics and predicted environmental concentrations can be utilized within the ERA. With such interest in the DtD chemicals, it is not surprising that there has been a considerable amount of scientific advances to better predict the environmental fate of these types of chemicals. This proposed session will highlight the global advances in wastewater/watershed modeling and laboratory environmental fate studies, including the use of appropriate protocols and test conditions to more accurately reflect environmental conditions, leading to a more predictive paradigm for assessing the environmental fate of DtD chemicals. The speakers will not only illustrate the advances in the field, but will draw upon the historical environmental fate methodologies conducted for these DtD chemicals and elucidate why some of the current tests (e.g. ready biodegradation test) may not be useful. Session attendees will come away from this session with a detailed knowledge of the limitations of the current methodologies, as well as the new methodologies to overcome these limitations.

Highly Hydrophobic Chemicals: Reliable Investigations on Environmental Fate and Effects

Felix Stibany, Philipp Mayer, Stefan Trapp, Kilian Smith

May 10, 8:35 - 10:15, The Arc

Highly hydrophobic chemicals with very low aqueous solubility are used in a broad range of applications ranging from personal care products to heavy industry. Large numbers of substances with $\text{Log Kow} \geq 5.5$ are already registered in the European Chemicals Agency (ECHA) database under the EU Chemical Legislation regulation. Further to their high production volumes, the release of these chemicals into wastewater and the aquatic environment cannot be precluded. Therefore, reliable assessments of the environmental fate and potential environmental toxicity are urgently needed for poorly soluble chemicals. However, investigations into their environmental fate and toxicity are not straightforward. Their high hydrophobicity results in extensive sorption to solids such as soils, sediments, organisms, and other surfaces. Therefore, standard tests for determining their toxicity or (bio)degradation that follow national and international guidelines are often not suitable for these chemicals. In particular, it can be challenging to provide defined and constant exposure concentrations in laboratory experiments but also to measure these concentrations. This is even more difficult when attempting to measure the exposure concentrations in the environment. The lack of consistent and reliable results due to these difficulties can lead to improper assessment of their environmental risks. Additionally, there are ongoing discussions about the presence of a general aqueous toxicity threshold (i.e., no toxicity below a certain concentration) or a general hydrophobicity toxicity cut-off (i.e., no toxicity above a certain Log Kow). Reliable toxicity data in the high Log Kow range are therefore urgently needed to clarify this issue, which in turn requires improved testing methods. Bioconcentration kinetic models and thermodynamic concepts will also be needed for setting and challenging such cut-offs. This session will discuss the above issues by addressing the following questions: What are adequate methods for a reliable assessment of fate and effects of highly hydrophobic chemicals? How can the present guidelines be improved to arrive at a more reliable assessment of the fate and effects of highly hydrophobic chemicals? What are the impacts of sorption on the toxicity and biodegradation of highly hydrophobic chemicals under realistic conditions? How can the fate and effects of highly hydrophobic chemicals be modelled and predicted?

In situ measurement of nanoparticles

Geert Cornelis, James Ranville

May 8, 8:35 - 10:15, Gold Hall

The quest for the limits of in-situ measurements of nanoparticles in environmental and biological samples and implications for modelling Measurement and characterization of engineered nanomaterials (ENM) has revolutionized over the past decade. While initial efforts have mainly focused on characterizing size in stock suspensions of predominantly ENM, we now have tools at our disposal to also characterize other relevant measurands of ENMs such as shape and number concentration, often at environmentally relevant concentrations and in difficult biological and environmental matrices where that was previously impossible. Development of single particle ICP-MS has been instrumental in this evolution, bringing a technique to maturity that is now routinely capable of measuring size and number concentration of inorganic ENMs in a wide range of environmental samples. Having these opportunities, however, it is still unclear how they can validate models being developed for environmental fate of ENMs. Bridging the gap between measurement and modelling is still an active area of research, where both model predictions need to be in line with what can be measured and measurement techniques become more in line with required model measurands. This session is seeking abstracts that are specifically facing these challenges. Priority will be given to new or refinement of existing techniques that widen the realm of possibilities to analyse ENMs in-situ in difficult biological and/or environmental matrices and attempts to bridge the gap between measurement and modelling.

Insights and challenges concerning the bioavailability of organic chemicals and communication implementation in risk assessment

John Parsons, Jose-Julio Ortega-Calvo, Jörg Römbke, Joop Harmsen

May 9, 8:35 - 10:15, Meeting Studio 313 & 315

The bioavailability of organic chemicals in soil and sediment is an important area of scientific research. In some cases, regulators have recently started to consider bioavailability within retrospective risk assessment frameworks (e.g. of historically contaminated sites) for organic chemicals; by doing so, more realistic decision-making in terms of hazard definition and priority considerations can be achieved than by relying on the established approach of using total-extractable concentrations. However, implementation of bioavailability concepts remains difficult because scientific developments are not always translated into ready-to-use approaches for regulators. The main objective of this Session is to discuss recent developments in this field and to identify and provide scientifically-based solutions to the challenges faced by regulators and industries in considering bioavailability issues during risk assessment, regulation and remediation of sites contaminated with organic chemicals. This session will build upon the developments outlined in a recent position paper (Ortega-Calvo et al. 2015) that was published in *Environmental Science and Technology* From Bioavailability Science to Regulation of Organic Chemicals, <http://pubs.acs.org/doi/abs/10.1021/acs.est.5b02412> as well as a new ISO standard 19204 (2016). This session will provide a discussion forum for existing bioavailability concepts and methods, options for their innovative application and standardization, as well as pathways for their implementation into retrospective risk assessment, regulation and remediation. Papers will be welcome on the different perspectives and interests on bioavailability: whether the focus is on soils, sediments or waters; on methodological issues (e.g., chemical and biological methods for measuring bioavailability); on communication needs (message simplification, verification); or if, finally, the motivation is to look at bioavailability-oriented remediation strategies (e.g. bioremediation, use of sorbents).

Measuring and Estimating Dose Metrics: Linking Exposures to Effects for improved Chemical Risk Assessment

Todd Gouin, Steven Droge, Beate Escher, Philipp Mayer

May 11, 8:35 - 10:15, Meeting Studio 313 & 315

The objective of chemical risk assessment is to ensure that exposure to chemicals in the environment and to humans does not result in adverse effects. To determine the likelihood of an adverse effect (e.g. toxicity) to occur, three components of the process must be understood: external exposure, toxicokinetics (TK), and toxicodynamics (TD). For external exposure, a number of physical, chemical, and biological factors influence the bioavailability of a chemical in the exposure media. Similar factors also influence how a chemical is distributed within an organism or the human body (TK), where processes such as biotransformation and elimination compete with factors influencing the distribution of a chemical to a site of toxic action. A fraction of the absorbed dose reaches the target or sites of toxic action, where this target dose (also called biologically effective dose) initiates a chain of biochemical reactions influencing the TD associated with the adverse effect observed. Although the exposure dose is fundamental to accurately defining dose-response relationships associated with a specific toxicological response, the biologically effective dose at the actual site of toxic action is typically not quantified directly; only surrogate dose measurements, total internal concentration or calculated target site doses can be obtained. A key component towards improved understanding of the dose-response relationship relies on better tools that can quantify the freely dissolved concentration (C_{free}) both in the external environment and internal tissues, organs, and cells of organisms or within in vitro test systems. A key objective of this session is thus to highlight advances in both modelling and measurement techniques aimed at quantifying C_{free} and cellular concentrations; this would include analytical methods aimed at characterizing the partitioning and binding behaviour of chemicals to various environmental and biological matrices, developments in mechanistic TK and TD modelling tools, and application towards quantitative in vitro to in vivo extrapolation corresponding to adverse outcome pathways.

Metals in the Environment: Fate, Speciation and Bioavailability in Water, Soil and Sediment

Erik Smolders, Karel De Schamphelaere, Christopher Cooper

May 8, 8:35 - 16:00, Copper Hall

While over the past two decades knowledge about metal transport, distribution, speciation and bioavailability has considerably increased and while this knowledge has begun to find its way into environmental regulation of metals, metals environmental science keeps progressing and novel scientific and regulatory questions arise. This session will welcome all contributions about fate, chemical speciation and bioavailability of cationic metals, organometals or toxic oxyanions in the environment. It will cover water, soils and sediments, will include fate modelling and observations, environmental chemistry of metals and bioavailability of metals across different species and exposure routes. We welcome novel contributions for this field of research.

Modelling and monitoring of pesticides fate and exposure in a regulatory context

Bernhard Gottesbueren, Christina Pickl

May 8, 11:05 - 16:00, Hall 300

Modelling and monitoring of fate and exposure of pesticides (incl. biocides) in the regulatory context is under continuous development in Europe as well as other regions of the world. Development of new models or the adjustment of existing models like changes in parameterization or scenarios are necessary due to new scientific knowledge and aim to a more reliable risk assessment for regulatory decision making regarding the protection of the environment whilst significant uncertainties remain. Monitoring campaigns of chemicals and metabolites are initiated to evaluate chemical status in different environmental compartments, whereas the questions on the regulatory context and implications of findings remain. The session will a) focus on the outcomes of recent developments on fate modelling under different regulations like new guidance documents, requirements and model developments. For example new guidance documents and scientific opinions on exposure assessment in soil, groundwater and surface water of pesticides have being developed by the European Food Safety Authority (EFSA). These shall be presented to and discussed by stakeholders from academia, regulatory authorities, industry and consultancy. For biocides, the European Chemicals Agency (ECHA) have the role of coordinating the European peer review process and have an increasingly important role in the associated development of risk assessments and emission scenarios documents in this area. New model or scenario developments shall be presented considering the spatial and temporal variability of the exposure and fate of pesticides in different environmental compartments. b) look at other regions of the world environmental risk assessment schemes, including modelling and their current developments and/or revisions (for pesticides e.g. in China, Latin America). A global exchange on exposure assessment principles (including modelling and scenario development) is warranted and it is the intention to bring together the latest developments in the regions of the world for different use classes of chemicals. c) provide a platform to discuss and exchange monitoring programs and results in the light of regulatory use. Modelling results shall be compared to monitoring data in order to allow an evaluation of their conceptual basis in relation to protection goals, which quite often may only be implicit in the underlying legislation. The regulatory use of fate models and scenarios for pesticides shall be discussed in the light of targeted experiments or representativeness analysis as well as survey monitoring results. The suitability of generic regulatory exposure scenarios and the development of tailor made scenarios shall be discussed alongside rules for their evaluation in a regulatory framework. As the scope of this session covers various chemical use classes, it is intended to focus the contributions in subsections, which are specific enough to attract the specialists but are linked and associated to foster the exchange between different scientific and regulatory communities.

Nanomaterial fate and toxicity - Implications of the environment as a global reactor for nanomaterials along their life-cycle

Susana Loureiro, Claus Svendsen, Kees van Gestel, Iseult Lynch

May 8, 11:05 - 16:00, Gold Hall

Nanomaterials (NM) enter the environment through direct application, runoff from fields to aquatic systems, recreational activities, and waste water treatment plant effluent and sludge, among others. During the application, the emission and the treatment, and in the environment, NM undergo several changes and reach biological targets in complex forms with altered properties compared to the pristine NM. In contact with organisms, NM can change their structure and proceed their life-cycle again in a different form. Therefore, it is crucial to understand processes that modify the properties of the NM and to what extent the environment acts as a global reactor, consisting of several small-scaled reactors. It is important to assess impact of the transformations of NM on their environmental fate and speciation, which adds more complexity to the evaluation of hazard and risk of NM. This session, therefore, aims at covering studies related to changes of NM properties along their life cycle. This includes changes of NM induced by i) emission from bulk materials, ii) waste water treatment, iii) reactions within different environmental compartments such as soils and surface waters, vi) interactions with soil and aquatic microbiomes, plants, invertebrates and vertebrates. Processes that change NM properties and consequently affect their environmental fate and speciation will affect the exposure and toxicity of NM to organisms. The concept of eco-corona is a key-aspect in understanding how the formation of a biomolecule corona changes NM properties and consequently the way NM interact with organisms. Toxicokinetic and toxicodynamic modelling will provide a vital input when looking at biota as a bio-reactor that can induce speciation changes or store nanomaterials in a less harmful form.

Organic micropollutants in the environment: analytical challenges and engineering innovations

Kristof Demeestere, Lynn Vanhaecke

May 10, 11:05 - 16:00, The Arc / May 11, 8:35 - 12:45, Silver Hall

Advances in analytical chemistry have resulted in the discovery of an increasing number of anthropogenic emerging organic contaminants in the environment, such as pharmaceuticals, pesticides, sunscreen/ultraviolet filters, artificial sweeteners, brominated flame retardants, perfluorinated compounds, PAH-derivatives, benzotriazoles, benzothiazoles, plasticizers, surfactants, and disinfection byproducts. The detection of contaminants is most probably not an isolated case; rather the tip of the iceberg. The awareness grows that even more unknown contaminants and transformation products are dispersed in the environment. This continuous burden on the environment of organic micropollutants with often an intrinsic ability to interfere with organisms concerns the scientific community. Additionally, increased use of reclaimed waste water (e.g. for crop irrigation) might expose human individuals to xenobiotics. Potential (eco)toxic effects can be a threat for the good status of ecosystems and human health. Analysis of trace concentrations of contaminants in the environment is challenging but prerequisite for studying and monitoring their fate and occurrence. Moreover, driven by pending (European) legislation and/or as a precaution to protect the environment, technological upgrades are needed to remove these micropollutants from waste streams. This session is looking for original oral and poster contributions to discuss latest progress in the field of research on (emerging) organic micropollutants in the environment. Topics include but are not limited to: - Trends and innovations in environmental analysis and monitoring of (emerging) organic micropollutants: both fundamental analytical research and field applications (e.g. sampling approaches, development and validation of analytical techniques, target and non-target screening, effect-oriented analysis, field monitoring,...) - Environmental fate and behaviour (e.g. environmental occurrence of newly detected organic micropollutants, partitioning and degradation in the environment, trends in monitoring data,...) - Technological developments and strategies to mitigate in a sustainable way organic micropollutants in the environment (e.g. improvements and innovations in abatement technology, reaction pathways, chemical and biological assessment, experiences with pilot- and full-scale installations, process control and process integration,...) - The way forward: innovative proposals for adaptation and updating of existing monitoring and engineering approaches taking into account the socio-legislative-economic context.

Persistence & Biodegradation Assessment

Thouand Gerald, Graham Whale, Jacques Lharidon, Arnaud Boivin

May 8, 14:20 - 16:00, Meeting Studio 311 & 312

The ability of certain chemical substances to persist in the environment requires careful consideration for the regulatory evaluation of environmental risk and hazards (e.g. classification, labelling and PBT/vPvB assessment). Indeed degradation of organic chemicals in the environment influences exposure and hence, is a key parameter for estimating their potential long-term adverse effects on biota. Assessing biodegradation [as "the biologically mediated degradation or transformation of chemicals usually carried out by microorganisms" (ECHA, 2012)] is among the first steps to evaluate chemicals persistence. Biodegradation is a natural but still poorly understood process which outcome strongly depends on the various environmental conditions and the microbial diversity. Higher tier testing requires more complex and expensive simulation tests (e.g. OECD TG 303, 307, 308, 309 and 314) which are selected upon the environmental compartments of concern (wastewater treatment plants, surface water, sediment or soil). Assessing chemicals persistence in the environment is still a challenging domain and there are different ways of addressing the issue depending on the regulatory context: Chemicals, Agrochemicals, Biocides, or Pharmaceuticals which may sometimes lead to conflicting results. For example the new temperature of 12°C for degradation tests under REACH Regulation may lead to consider some substances as being persistent although they were not considered as such. In addition, the PBT Guidance document within REACH Regulation has just started a formal revision process where the latest developments in the area should be considered. The characterization of the microbial diversity, the bioavailability of test substances in standard screening assays, the test design in water-sediment degradation tests, the way to combine field tests, abiotic degradation processes, simulation tests in waste water treatment plants are all examples of topics where recent results need to be taken into account for Regulatory purposes. Beside these regulatory considerations, the session will give the opportunity to present technical and scientific developments in the different fields associated with persistence and biodegradation assessment (e.g. investigating the value of characterizing microbial biomass diversity through genetic sequencing, chemical mixtures degradation assessment, evaluation of non-extractable residues, new testing and measurement instrumentation, interpreting data to improve the relevance of testing strategies and Weight of Evidence approaches for persistence assessment).

Poly- and perfluoroalkyl substances (PFASs): Recent developments, sources, transport, fate and toxicity

Lutz Ahrens, Zhanyun Wang, Annegret Biegel-Engler, Ronald Bock

May 8, 8:35 - 12:45, Meeting Studio 311 & 312

This session focuses on the recent developments in the field of legacy and alternative poly- and perfluoroalkyl substances (PFASs) and how these developments contribute to the understanding of the big picture. Specifically, this session puts emphasis on those emerging and novel PFASs for which analytical methods are lacking and whose properties, exposure and risks are still being investigated. We particularly welcome contributions within the following areas: i) development of new analytical techniques (e.g. alternative PFASs, total organic fluorine, total oxidation, and other non-target analysis), ii) improved understanding on their intrinsic properties including physicochemical properties such as partitioning behavior, degradability and degradation pathways, bioaccumulation behavior such as mechanism, tissue distribution and maternal transfer, and toxic effects on wildlife and humans, iii) importance of assessing alternatives in light of their efficiency and usability by end-users, iv) improved understanding on the environmental and human exposure to PFASs including their sources and occurrence, fate and transport processes, exposure routes, associated risks, and epidemiological evidence, v) latest developments on treatment methods to identify and remediate contaminated sites, and vi) risk management and options for regulation. Ultimately, the session aims to highlight recent milestone research, identify critical knowledge gaps and provide a roadmap for future research.