Advances in exposure modelling: bridging the gap between research and application

Chairs: Antonio Franco, Emma Undeman

Environmental fate models are widely used to investigate transport and fate processes as well as to estimate chemical concentrations in air, soil, water, sediment and biota. Although their use has long been established in both research and regulatory practice, the wider range of chemicals under scrutiny, including substances with "unusual" properties, and the quest for increased ecological realism in higher tier exposure assessment are pushing the boundaries of traditional modelling approaches. For instance, novel modelling techniques have been developed for contaminants such as metals, engineered nanoparticles, ionizable or surface-active organic substances and other chemicals to account for their specific speciation, phase partitioning and intermedia mass transfer mechanisms. GIS-supported, spatially explicit models have enabled enhanced parameterization of spatial-temporal variability of biotic and abiotic parameters influencing partitioning, transport and bioavailability. However, these models require high-resolution spatial (and temporal) data for parameterisation, which is often unavailable or difficult to retrieve. An additional challenge relates to the development of tools to estimate chemical emissions, both for screening and higher tier assessments. The integration of contaminant fate models with atmospheric, hydrological, biogeochemical and ecological models adds realism to simulated scenarios, although at the cost of increased complexity. Lastly, the application of recent advances in modelling tools for chemical risk assessment and management remains challenging, particularly in the regulatory context. Systematic model evaluation is one of the main barriers. Coordinated monitoring and modelling efforts are most beneficial for both monitoring design and model development.

This session focuses on recent development in exposure modelling. Particularly welcome are studies that address scientific and regulatory challenges towards the implementation of advanced modelling techniques for chemicals risk assessment and management. Topics of interest include the extension of the chemical domain of applicability, methodologies to estimate chemical emissions, spatial and temporal explicit models, the integration of multidisciplinary models, the design and coordination of monitoring activities for parameterization and evaluation of models, sensitivity and uncertainty analysis, and generally the implementation of good modelling practice in the development, evaluation and use of exposure models.

Sponsored by: Exposure Modeling Advisory Group (Global)

Preliminary session type: Platform and Poster

An in silico modelling perspective to advance hazard assessment of aquatic ecotoxicology

Chairs: Paul Thomas, Malyka Galay Burgos, Charles Eadsforth

The applications of in silico approaches such as Quantitative Structure Activity Relationships (QSARs) and Read Across are well known for predicting several endpoints of environmental concerns. The usefulness of such methodologies is more evident in the absence of validated test guidelines or to overcome the limitations of available test methods to handle a wide range of chemical substances. However, there had been several concerns over their reliable use for regulatory purposes mainly due to the lack of availability of validated data and the uncertainty associated with the model's output. However, things have considerably improved since the OECD principles for QSAR model validation was implemented and QSAR reporting formats were made available for REACH purposes. Such measures have increased the recognition of the importance of in silico models as a serious alternative to experimental testing.

This session is aimed to highlight the usefulness of in silico alternatives to advance hazard assessment in the field of aquatic ecotoxicology. Poster and platform presentation abstracts are welcomed and authors are encouraged to address one or more of the below-mentioned topics relevant to enhance the role of in silico modelling towards the ecotoxicological assessment:

a) Development of reliable approaches to predict the aquatic toxicity to mixtures.

b) Better understanding of the Acute to Chronic toxicity Ratio (ACR) in the aquatic organisms.

c) Usefulness of Mode of Actions (MoA) and chemical activity concepts in ecotoxicological assessment.

d) Grouping and Read Across of ecotoxicological data.

Preliminary session type: Platform and Poster

Combining exposure and effects models and data for landscape based risk assessment in a regulatory context

Chairs: Mark Egsmose, Gerhard Goerlitz, Anne Alix, Katja Knauer

Environmental risk assessments (ERA) are an essential part of regulatory dossiers in support of the evaluation of regulated chemicals, such as pesticides, biocides and other chemical substances. ERA is performed in order to meet agreed specific protection goals, which provide the framework for carrying out the ERA as well as decision making criteria. Modelling, such as population models as well as appropriate monitoring data can be used for linking exposure and effects when applying landscape approaches. The availability of EU wide data eg appropriate monitoring data can be used for linking exposure and effects. It offers possibilities for moving to more complex landscape level assessments to refine ERA as a supplement to standard lower tier assessments and allows to put the outcome of a risk assessment in perspective regarding the scale (spatial and time) of risk occurrence. On the other hand it creates a rising need to combine exposure with effect models and data and include the effects of multiple stressors. The effects caused by the exposure of organisms to toxicants depends on the configuration of the spatio-temporal concentration patterns of the toxicant in the environment on one side and on the behaviour and state of the organism on the other side. This makes the ERA especially complex when concentration patterns vary significantly over time and/or space. TK/TD models and population models can help to investigate the effects of complex exposure patterns on different levels of biological organisation from individuals to populations. These exposure and effect aspects must be combined in a realistic risk assessment. This session invites papers on:

- The ecotoxicologically relevant type of concentration (ERC)
    - -Dependence of the ERC on environmental compartment, species and stressors of concern
    - -How to address exposure to different toxicants (mixtures and repeated exposures in space and time)?
- Spatio-temporal configuration of toxicants and organisms in the environment
- How to combine different spatial and temporal scales and biological organizational levels in risk assessment?
    - -Toxicokinetics and toxicodynamics
    - -Individual organisms
    - -Populations
    - -Mechanistic exposure models
    - -Data and mapping generated at the landscape scale
- Calibration and validation of models/risk assessments spanning different spatial and temporal scales or organizational levels

Finally - while not directly part of the scientific discussion - contributions describing how risk managers can use landscape based risk assessments and risk assessments involving multiple stressors in decision making are encouraged since these would be essential for risk assessors and scientists to develop tools and instruments which can effectively support the decision making process.

Sponsored by: Mechanistic Effect Models for Ecological Risk Assessment of Chemicals (Europe)

Preliminary session type: Platform and Poster

Documentation and evaluation of mechanistic effect models for regulatory purposes: a first feedback from submitters and evaluators

Chairs: Udo Hommen, Maria Arena, Virginie Ducrot

Over the last years immense progress has been achieved in the development of Mechanistic Effect Models (MEM) to predict effects of chemicals on non-target organisms, populations and ecosystems. Guidance on good modelling practice as a tool for risk assessors to assess the usefulness of MEM in a specific regulatory context and for decision support has also progressed fast. The proposed session aims a getting a first feedback from scientists (i) which submitted models to support environmental risk assessment (ERA) of chemicals (e.g. for pesticides, biocides, pharmaceuticals and industrial chemicals) and (ii) which evaluated a submitted model in the ERA context. So, this session will not address the development and the description of new models or modelling approaches but it will focus on experience of modellers with e.g. meeting requirements from the Good Modelling Practice Scientific Opinion by EFSA when building and documenting their models (using e.g. TRACE or another documentation framework and experience of evaluators (especially regulators) with submitted models and their application. Feedback is welcome on submitted modelling approaches (number of submissions, types of submitted models, etc.), on experience in using the Good Modelling Practice Scientific Opinion by EFSA when evaluating models and assessing model documentation. In addition, contributions on experience with the evaluation of the regulatory relevance and of the quality of the model applications are also considered of interest, e.g. whether the model (and the chosen environmental scenario) was fit for the purpose of ERA with respect to the Specific Protection Goals and whether it provided robust, reliable results that could support concrete ecological risk assessment. In this respect, a discussion on the extent to which a model should (and can) be tested by comparison with real data, and on the acceptance of other validation methods (e.g. pattern oriented modelling) is also relevant.

Sponsored by: Mechanistic Effect Models for Ecological Risk Assessment of Chemicals (Europe)

Preliminary session type: Platform and Poster

Ecological modelling for risk assessment: state of the art, applications, and future directions

Chairs: Pernille Thorbek, Veronique Poulsen, Volker Grimm

Ecological modelling for risk assessment has undergone fast development in the recent decade and standards for design, documentation and testing have improved considerably. Modelling at different scales is entering regulation for pesticides e.g. honeybees (1, 2) and non-target arthropods (3), and guidance for good modelling practice has beendeveloped (4). However, since risk assessments of different species groups in different environments operate at different spatial and temporal scales and need to cover a wide range of regions and crops scenario, development and application of appropriate ecological models remains a challenge. Here, we take stock and invite studies to showcase state-of-art in effect modelling, application to risk assessments with special focus on scenario development, as well as studies outlining how model design and scenario development can be integrated.

References:

1. EFSA, EFSA Journal 11, 3295 (2013).

2. EFSA, EFSA Journal 13, 4125 (2015).

3. EFSA, EFSA Journal 13, 3996 (2015).

4. EFSA, EFSA Journal 12, 3589 (2014)

Sponsored by: Mechanistic Effect Models for Ecological Risk Assessment of Chemicals (Europe)

Preliminary session type: Platform and Poster

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

Chairs: Bernhard Gottesbueren, Lisa Hammond

Modelling of fate and exposure of pesticides and biocides in the regulatory context is under continuous development in Europe as well as other regions of the world encountering different regulations, guidance documents and requirements.

For example new guidance documents and scientific opinions on exposure assessment in soil, groundwater and surface water of pesticides are being developed by the European Food Safety Authority (EFSA). These need to 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 scientific risk assessments and emission scenarios documents in this area.

In other regions of the world environmental risk assessment schemes, including modelling, are under development and/or revision (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 of this session to bring together the latest developments in the regions of the world for different use classes of chemicals.

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.

New model developments shall be presented considering the spatial and temporal variability of the exposure and fate of pesticides and biocides in different environmental compartments. The development of environmental scenarios is fundamental for the exposure and risk assessment and shall be covered.

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 and biocides shall be discussed in the light of targeted experiments 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.

Preliminary session type: Platform and Poster

Quantitative in vitro to in vivo extrapolation (QIVIVE): Advances in tools to quantify exposure (dose)-response relationships and use in risk assessment

Chairs: Todd Gouin, Jon Arnot

High throughput in vitro toxicity testing is creating large databases of toxicity and bioactivity information. These data can be used to improve mechanistic understanding of toxicity pathways and for chemical assessments (e.g., screening and prioritization). The use of in vitro toxicity data in risk assessment requires quantification of exposure and tools for extrapolating between in vitro and in vivo systems. The National Academy of Science 21st Century vision for exposure science suggests a strategy that incorporates an integrated approach for the source-to-receptor continuum over multiple levels of integration to multiple stressors. A continuing challenge associated with the assessment of human and ecological risks associated with the use of products and chemicals are the data gaps and uncertainties quantifying internal exposures near, or at, the assumed site of toxic action from external exposures. Toxicokinetic (TK) models have been developed for various species and can include key processes such as absorption, distribution, metabolism (biotransformation), and excretion processes, i.e., "ADME". TK models can be developed empirically or from physiologically based data sets. The models can be single compartment or multi-compartment. The TK models typically require measured or predicted data for the organism and the stressor (e.g., partitioning and reaction properties). Advances in TK models and related parameterization tools specifically aimed at quantifying in vitro-to-in vivo extrapolation (QIVIVE) are critical for combining and comparing exposure estimates with in vitro toxicity testing data streams. Such tools can be used in a traditional "forwards" manner for exposure assessment and in a "reverse" manner for QIVIVE. The purpose of this session is to communicate advances in exposure and risk assessment as they relate to the development, evaluation and application of quantitative tools to help link the external and internal free concentration exposures with exposure (dose)-response relationships and strengthen QIVIVE approaches that can be used in regulatory risk assessment.

Sponsored by: Exposure Modeling Advisory Group (Global)

Preliminary session type: Platform and Poster

Recent Developments and Current Issues in Bioaccumulation Assessment

Chairs: James Armitage, Caren Rauert, Katrine Borga

Bioaccumulation is the net result of competing rates of the uptake of chemicals into an organism from the ambient environment and its diet and the elimination of chemical from the body via various processes. Assessment and categorization of bioaccumulation (B) potential is a typical requirement of national/regional regulations (e.g., REACH) and international agreements (e.g., the Stockholm Convention on Persistent Organic Pollutants) on chemical management. Many categorization schemes still rely heavily on the octanol-water partition coefficient (KOW) and bioconcentration factors in fish (BCF) for assessment purposes. Other metrics for bioaccumulation assessment, such as the bioaccumulation factor (BAF), biomagnification factor (BMF), biota-sediment accumulation factor (BSAF), trophic magnification factor (TMF) and total elimination half-life (t1/2) have also been proposed. Experiences with chemicals such as β-hexachlorocyclohexane (BCF < 2000 L/kg in fish, BMF > 1 in terrestrial and marine mammals) have demonstrated the need for weight of evidence (WoE) approaches for B assessment in order to incorporate and integrate various types of information that may be available. Besides the aforementioned 'BCF-BMF discrepancy' for β-hexachlorocyclohexane, there are other situations where B metrics may appear to be contradictory (e.g., BCF > 2000 L/kg, BMF, TMF < 1). A key process influencing B potential (and the congruency in B metrics across food webs) is biotransformation. While knowledge about biotransformation of organic chemicals has been increasing over the past decades through in vivo data compilations, QSAR development, in vitro method development and quantitative in vitro to in vivo extrapolation (Q-IVIVE), further work is clearly required. The objective of this session is to highlight recent research that can be incorporated in WoE approaches for assessing bioaccumulation in aquatic and terrestrial environments including analyses of laboratory and field data and the use of in vivo, in vitro and in silico methods. Case studies are welcome as are informed perspectives on the regulatory implications of apparent discrepancies and/or uncertainties in bioaccumulation data compiled during B assessments.

Sponsored by: Bioaccumulation Science Advisory Group (Global)

Preliminary session type: Platform and Poster

Spatiotemporal extrapolations in environmental risk assessment

Chairs: Michiel Daam, Antonio Nogueira, Carlos Barata

Given the natural variability in ecosystem structure and functioning, it is reasonable to question the extrapolation of environmental risk assessments in space and time. In addition, test compound exposure in ecotoxicology testing (e.g. single-peak and chronic) usually do not mimic realistic time-variable exposure regimes likely to occur in the field. On the other hand, it is neither financially nor practically feasible to test all ecologically relevant exposure scenarios (e.g., pulsed, intermittent, or chronic) on a large number of species and communities during different time periods. Therefore, both the extrapolation across time-varying exposure regimes and the spatiotemporal extrapolation of ecotoxicological effect data are important issues in ecological risk assessment. Better predictive power from mathematical effect models considering such issues can support policy and decision making and regulatory compliance. This session invites contributions dealing with extrapolations of study findings in both time and space. Presentations into extrapolations and modelling of causal links between anthropogenic pressures and ecosystem structure, functioning and/or services on higher levels of biological organization are especially welcome.

Preliminary session type: Platform and Poster