Speciation of PAHs in stormwater

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Published in:
Abstract Book

Publication date:
2012

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):

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Effects of repeated application of sulfadiazine-contaminated pig manure on abundance, diversity and activity of microbes involved in nitrogen transformation in different soil compartments.

ET19B-4
Effects of pig slurry co-applied sulfadiazine (SDZ) on the microbial diversity in soil microcompartments such as earthworm channels and rhizosphere soil.

ET19B-6
Effects of ivermectin application to cattle on dung fauna and dung degradation: an international comparison of field studies.

Modelling environmental risks of veterinary medicines used in Asian pond aquaculture

A kinetic model that couples environmental fate processes of antibiotics with an effect model of bacteria inhibition was studied. The model uses the antibiotics concentrations (disinfectant) in an intensive striped catfish (Pangasianodon hypophthalmus) scenario for the Mekong Delta (Vietnam). The ERA-AQUA decision support system can be integrated into a modelling framework to soil. The aim of this study was to investigate the effects of the antibiotic sulfadiazine in combination with pig manure on the abundance, diversity and activity of functional microbial communities involved in nitrogen (N) transformation in different soil compartments after repeated application of the antibiotic. The repeated applications of SDZ-contaminated manure to bulk soil entailed different responses of the functional groups involved in N cycling after the first, the second and the third amendments which might indicate an adaptation of the microbial communities to the antibiotic substance.

Effects of repeated application of sulfadiazine-contaminated pig manure on abundance, diversity and activity of microbes involved in nitrogen transformation in different soil compartments.

M. Schlotter

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Several studies from our group have indicated pronounced effects of single application of sulfonamide (SDZ) contaminated manure to soil. The aim of this study was to investigate the effects of the antibiotic sulfadiazine in combination with pig manure on the abundance, diversity and activity of functional microbial communities involved in nitrogen (N) transformation in different soil compartments after repeated application of the antibiotic. The repeated applications of SDZ-contaminated manure to bulk soil entailed different responses of the functional groups involved in N cycling after the first, the second and the third amendments which might indicate an adaptation of the microbial communities to the antibiotic substance.
ET19B-5

In vitro effects of 17β trenbolone on the mRNA levels of steroid hormone receptors, Growth Hormone and gonadotropins in pithitary glands from rainbow trout (Oncorhynchus mykiss)

University of Southern Denmark, Odense, Denmark

Based on the high biological activity of trenbolone in fish and on the uses done by bodybuilders, the compound might potentially pose a risk to the aquatic environment also in EU although not officially present. Previous studies in our laboratories have shown that trenbolone is capable of irreversibly changing sex ratios to 100% males in zebrafish at water concentrations in the low ng/l level. The present study was undertaken to investigate effects of trenbolone on mRNA levels of steroid hormone receptors, GH, LH and FSH in pithitary glands from rainbow trout after in vitro incubations of the excited tissues with the synthetic androgen.

GF-1 and AR mRNA levels in liver slices incubated with trenbolone at concentrations from 5-100 ng/ml were unchanged.

Pithitary glands were incubated with trenbolone from 1.35-1355 pg/ml:
- No significant changes were found in GH mRNA levels
- AR mRNA was significantly reduced at all concentrations
- FSH mRNA was significantly increased at the highest concentration
- LH mRNA was massively and inversely reduced with incubation concentrations

LC01 - Development in life cycle inventory analysis and modelling

LC01A-1

Market-based allocation of recycling benefits

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Market-based allocation of recycling benefits has already been described since the years 2000. However, this approach tends not to be largely adopted in international standards.

In practice, there are mainly three types of benefit allocation with system expansion modeling: (i) allocation of benefits to the producer bringing material on the market (that can be defined as the secondary material at end-of-life); (ii) allocation to the product incorporating secondary material and (iii) 50/50 allocation (half of the benefits of recycling at end-of-life and half of the benefits of incorporating secondary material are accounted for).

Market-based allocation is dictated by the answers to the following questions: "Which additional amount of secondary material will be exchanged on the market if supply increases thanks to the apparition of a new source of secondary material?" or "Which additional amount of secondary material will exchanged on the market if demand increases thanks to the apparition of a new producer of a good based on the secondary material?" Analysis of a price elasticity of demand and supply provides answers.

This paper aims at depicting several typical supply-demand curves and at associating these to actual market situations (for example, what if there is a back obligation or subsidized waste collection, etc.). The appropriate market-based allocation can hence be dictated in each case.

Namely, allocation to the supplier (i) is to be promoted in cases where the supply is fully inelastic and where the demand is fully elastic. Examples of such markets are, among others, PET and packaging gas.

In markets where answers to supply and demand variations are more equilibrated, a 50/50 allocation should be used, as it is the case for certain types of paper and boards.

Market situations for main materials are analyzed so as to provide sound justification for standard developments.

LC01A-2

Using a long-term energy model for the consequential and prospective life cycle assessment of the use of biomass based synthetic diesel (BTL) in France

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Consequential Life Cycle Assessment (C-LCA) has been developed recently as a modeling approach that captures environmental impacts of a product beyond direct physical relationships accounted for in Attributional LCA. This approach seems interesting for the evaluation of biofuels since their indirect impacts on other sectors (agriculture, forestry, electricity production) may be important. In this study, we use a prospective optimization model representing the French energy production and transportation sectors (agriculture is partially included due to the presence of biofuels) to evaluate the impacts of the production of BTL in France in the time horizon 2007-2030. The model was developed with the economic model generator TIMES.

Part of the work consisted in adapting the model to perform C-LCA integrating energy consumptions and emissions factors to the technologies described in the model. Scenarios were built in order to expose the C-LCA methodological issues we aim to discuss. We observed how the model behaves when applying variations to: the technology used for BTL production, the levels of development of LCA in France and the energy policy. Global Warming Potential (GWP) was calculated for each scenario using time-dependent characterization factors for greenhouse gases.

Preliminary results show that the long-term energy model can be applied for measuring the indirect effects of the development of BTL in France. For example, it was possible to identify the source of the electricity that is going to compensate the supplementary demand for electricity due to the production of BTL using an allometric process. This type of model presents some advantages in relation to other models previously used in C4-LCA:
- It allows a fine description of transformation steps of primary resources in energy carriers.
- It allows the observation of marginal and non-marginal perturbations on the energy sector.
- Emissions are exogenious to the model. Most of the other C-LCA studies use economic equilibrium models to quantify the consumption of certain products and the emissions are integrated manually afterwards.

Nevertheless, in this version of the model, the agricultural sector is only described partially and land use changes (direct and indirect) can’t be evaluated. A whole world description of the agriculture and forestry sector would be necessary for this type of analysis. One way of improving this C-LCA would be to integrate our model with a general equilibrium model.

LC01A-3

Modelling land use changes in consequential LCI: limitations of equilibrium models

1Public Research Centre Henri Tudor, Luxembourg-kirchberg, Luxembourg
2Ordecsys, Chêne bourg, Switzerland
3Public Research Centre Henri Tudor, Luxembourg-kirchberg, Luxembourg

This presentation aims at discussing the use and limitations of economic equilibrium models for the development of consequential LCI, with a specific focus on the case of biomass production from maize in Luxembourg. The core research objective is the development and application of a Partial Equilibrium (PE) model representing the market constraints and reaction to the demanded production of maize and providing: 1) the change of crop production patterns, i.e. the primary consequences on Luxembourg's agriculture system. Forage crops are included, making the link to the consequences on meat and milk production. 2) The changes of land use type and related primary consequences in terms of modified pollutant emissions and land transformation impacts. The modelled changes are then propagated inside the national economy, using a general equilibrium model for Luxembourg (IFP Energies nouvelles) and outside the national boundaries to account for additional environmental impacts.

So far the results show no need for intensification of the existing and new areas to meet demand for maize. To study the impacts of increased agriculture prices, we increased the import prices of the "agriculture" commodity by 10% in Luxemmburg calibrated to the base year 2005. We find that the share of expenditure by households on agriculture products increases thanks to the apparition of a new source of secondary material. Agricultural land use changes in the value added in the economy and increased demand for maize which may displace existing crops will not have serious economic impacts. These findings were corroborated using the global model GTAP, which was used to evaluate the increased demand for displaced agriculture crops on account of additional production of maize. However, since the PE model is based on revenue maximization, it is difficult to properly consider non-economic constraints such as behaviours related to habits, cultural heritages or additional regulatory constraints. Also the modelling of the influences of crop production patterns on the food sectors is not trivial because of the difficulty of assigning a clear and robust aggregated market relation between forage crops and meat and milk.
Equilibrium models fall short in including technical and non economical constrains. The complementary use of agent-based modelling could be an alternative approach for proper consequential LCI.

LC01A-4 Integrating accident-related methods and impacts into the life cycle toolbox
M.A. Wolf
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Life cycle Assessment presupposes the need to understand more to be 'only' one component of a wider environmental and even sustainability assessment toolbox. Enhancing classical Life Cycle Inventory (LCI) modelling by integrating accidents in production, use and end-of-life of products is one important step towards more complete evaluation of product systems' life cycles. LCA according to ISO 14040ff deals implicitly with non-accidental ('regular') releases only, while some accidental releases may be included due to how LCI data is collected (e.g. site's yearly average, including leakages etc.). There are however important organisational and decision-making related reasons for managing these two types of generation separately. Accident prevention in industry is done separately from dealing with normal releases to the environment. A separate inventory of accident related releases and casualties (Life Cycle Accident Inventory, LCAlI) is hence required for effective decision support. Several studies present case-specific solutions for this issue and some general method concepts have been presented. A systematic and consistent methodological solution for full implementation is still lacking. Joining LCI methodology and tools from Risk Assessment (Event Tree Analysis and Fault Tree Analysis) yields a powerful approach for integrated analysis of the environmental and health effects from accidents. This paper presents a methodological approach to how to reflect accident scenarios on consequential modelling principles when modelling accident inventories for joint analysis with LCI data. The presentation will systematically address the question of how best to place the accident-related impacts within the life cycle toolbox and which methodological implications this has. Data sources and data management are further issues to discuss to ensure a proper approach in support of life cycle based decision making in industry.

LC01A-5 Better characterising the environmental performance of intermittent power generation with help of LCA: integrating wind power into the German electricity grid in 2006
T.M. Bachmann, J. van der Kamp, R. Stermann
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Intermittent power generation and in particular wind power is continuously gaining shares in the power plant parks of many countries. Given its intermittent nature, however, the true environmental impacts increased wind power integration remain an open question. This is because the seemingly equivalent functionality expressed in a kWh of electricity produced is in fact not directly comparable across systems. For this reason, a more systemic approach is advocated. Relying on energy systems analysis results, the purpose of the study is to analyse to what extent considering substitutional effects and back-up can help characterise power generation from intermittent resources. The study starts with describing the German electricity grid in 2006 with and without wind power generation. By using the results from an agent-based energy system model, the issues of intermittency and the backup needed for wind power were addressed. Through substitution of fossil fired capacities, the study is considering these consequences led to an even better environmental performance of wind power in all of the considered impact categories (including global warming) compared to the LCA not considering these, except for mineral resource depletion and natural land transformation. As this study could not fully resolve the issue of finding a functional unit that is more appropriate than the kwh for comparing different power generation techniques, other approaches are also discussed.

LC01B-1 Book, trade and claims LCA: how to model certificates delinked from physical flows
R. Frischknecht, R. Itten
ESU-services Ltd., Uster, Switzerland
In May 2011, the association of issuing bodies AIB announced that 1 billion EECS certificates (which equals 1 billion MWh of electricity) have been issued in Europe since its start nine years ago. There is a large demand in large renewable energy certificates, which help electric utilities and companies from the manufacturing as well as service sector to reduce the environmental impacts of the electricity they purchase.

The international standards on life cycle assessment (ISO 14040, ISO 14044) do not specify how certificates should be taken into account when performing a product or company's life cycle assessment (LCA) study. The recently come into effect carbon footprint standard are clear with regard to carbon offsetting measures (emission certificates); these are considered as an improvement measure and shall not included in the product LCA but kept separate.

Up to now, the role of renewable energy certificates has not been considered widely. This presentation shows the mechanism and volume of RECS certificates as well as its consequences on the LCA of electricity and how they may or may not be used within product LCA and other LCA studies.

During the last years, countries with large shares of hydroelectric power exported significant amounts of RECS certificates to other European countries. These RECS certificates are used to delink the carbon footprint of electricity purchased by companies and electricity providers. Thus the exports are compensated by imports of the same amount of non renewable energy certificates. This leads to substantially higher carbon intensities of the electricity mix of exporting countries.

We therefore recommend to disregard independently traded RECS certificates in product and service LCA as long as the LCIs of national electricity mixes is based on international statistics disregarding RECS trade. If RECS certificates are linked to the production and delivery of renewable electricity, we recommend to include the respective share of renewables in the electricity mix.

LC01B-2 Using water markets and consequential LCA to assess indirect impacts from water use
A.M. Boulay, C. Bulle, M. Margni
CIRAGE - Ecole Polytechnique de Montreal, Montreal, Canada
Using water can incur direct impacts on human health from water deprivation for domestic use or agriculture. However, these impacts do not occur in regions where economic resources are sufficient to allow the deprived users to turn towards technology to meet their needs. On the other hand, this technology leads to burden shifting that should be captured in a comprehensive assessment of water use in LCA. This paper proposes a consequential framework and model using water markets and marginal technology in order to assess LCA indirect impacts from water consumption and degradation, by identifying marginal processes and including their life cycle inventory. Adapting our approach to the given type of water withdrawn, defined by its source and quality, is constrained. The assessment whether a water type is constrained or not is performed through a scarcity parameter, with the underlying assumption that an unconstrained resource is not scarce. The market concept, applied to water, is then used for each water type to consider all sources for this water type. These include available water of this type, treated water from a lower quality source of water, desalinated water, and imported water. Additional water is associated with each of these source of water.

Results consist of quality-specific marginal water source available for 808 hydro-economic cells worldwide, as defined in Boulay et al, resulting in 6464 (808 cells x 8 water types) marginal processes which can then serve as input to the inventory and be assessed by any impact assessment methodology. Preliminary results are plotted on a world map giving additional energy demand incurred by the marginal processes for a 1000 m3 of good quality surface water use for each 808 hydro-economic cells.

This approach provides a first approach assessing indirect impacts from water use due to compensation scenarios. It is especially relevant for developed countries facing water scarcity and/or poor water quality by overcoming current methodological limitations that solely consider direct impacts on human health from water deprivation. This model is based on a consequential approach, identifying the unconstrained marginal source of water and treatment processes required to compensate the deprivation from water use.

LC01B-3 Modelling of biogenic CO2 fluxes in LCA and their integration with the global C cycle
F. Cherubini, A. Stromman
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In Life Cycle Assessment (LCA), the same characterization factors are conventionally applied irrespective of when the emissions occur (the same importance is given to emissions in the past, present and future). This accounting paradigm makes bioenergy systems climate neutral as long as they are carbon neutral (the same amount of CO2 releases from combustion is sequestered by growing trees). When the analysis is constrained by specific time boundaries the validity of this convention becomes shaky.

We stress the fact that the equivalency between C and climate neutrality in bioenergy LCA ignores the temporal gap between the emission (usually at a single point in time) and the sequestration flux, which is usually distributed over many years. Neglecting these dynamics has an influence on the final climate impact assessment. The challenge for LCA practitioners is to model these fluxes and calculate the resulting climate impacts with unit-based indicators that be included in LCA case studies.

In this work, we elaborate on this issue using relatively simple mathematical methods which provide simulations of the carbon flow dynamics of biomass systems. Probabilistic distribution functions are used to include in LCA the dynamic profiles of CO2 emissions and removals associated with biomass management for bioenergy and wooden products following an approach based on Impulse Response Functions, CO2 atmospheric profiles are calculated together with the respective changes in radiative forcing. Results show the importance of using emission and removal functions rather than single pulses or linear amortization procedures, which generally overestimate the climate impact of CO2 emissions, especially in presence of short time horizons and for relatively wide time-distributed emissions.

This set of flexible and can provide guidelines that are suitable to be routinely applied in LCA. Following this, we believe that a debate should be open in the LCA community to properly address timing of emissions and revisit the climate metrics used in the assessment. Besides normalized metrics as GWP, absolute metrics showing how the impacts change over time are preferable and can provide additional insights on the effective mitigation potentials of the system under study. The approach presented here deserves future research for a possible use in accounting of emissions from harvested wood products and in processing data by emission inventory experts within the Kyoto protocol and its successor.
Environment and society. This research aims at investigating the relationship between HL and LCA and at developing an operational framework to include HL in LCA. A framework for prospective hybrid life-cycle assessment and its application to energy technologies

Assessment (LCSA) tries to make a bridge between the traditional environmentally oriented and generic life cycle assessment (LCA) and the more site- and time-specific sustainability budget. Within the case studies, the HL significantly contributes to the total impact for several categories (e.g. fossil and ozone depletion up to 16% and 20%, respectively) that a qualified worker always generates impacts greater than other workers. The impact of average HL is higher in EU countries with the highest household expenditures' economy and society. This research aims at investigating the relationship between HL and LCA and at developing an operational framework to include HL in LCA. A framework for prospective hybrid life-cycle assessment and its application to energy technologies.

A framework for prospective hybrid life-cycle assessment and its application to energy technologies

A model of EU-27. Afterwards, ten agri-food and industrial LCAs case studies were modified for hybrid LCAs, adding HL inputs to existing LCIs. The LCIA comparison showed that a qualified worker always generates impacts greater than other workers. The impact of average HL is higher in EU countries with the highest household expenditures’ economy and society. This research aims at investigating the relationship between HL and LCA and at developing an operational framework to include HL in LCA. A framework for prospective hybrid life-cycle assessment and its application to energy technologies.

Scope

This publication describes life cycle techniques that can measure sustainability and allow LCA to support decision-making toward more sustainable product and process systems. An (Environmental) LCA looks at potential impacts to the environment as a result of the extraction of resources, transportation, production, recycling and use and discarding of products; life cycle costing (LCC) is used to assess the cost implications of this life cycle; and social life cycle assessment (S-LCA) examines their social implications related to and affected by, changes to the functional unit. Nevertheless, HL could be seen as the common numeraire among the three pillars of sustainability: environment, economic and social. This publication shows how all three techniques - which all share similar methodological frameworks and aims - can be combined to make the move towards an overarching LCSA possible. Conclusion LCSA has significant potential to be used by enterprises, governments, agencies for international cooperation and other organizations in society (such as consumers’ associations) in their efforts to produce and consume more sustainable Still more research and applications are needed, but its application is already feasible and encouraged to speed the learning curve of the society.

Challenges in implementing Life Cycle Sustainability Assessment (LCSA) and in an LCSA-based decision-making

Technical University of Denmark, Lyngby, Denmark Life Cycle Sustainability Assessment (LCIA) has been proposed to be a combination of three assessments: environmental, economic and social (incl. socio-economic). In this way LCSA tries to make a bridge between the traditionally environmentally oriented and generic life cycle assessment (LCA) and the more site- and time-specific sustainability assessment (SA), which takes into account all three generally accepted pillars of sustainability (economic, social and environmental). In the process of trying to bridge and to draw from the strong characteristics of SA and LCSA, LCA encounters its own challenges.

Life Cycle Impact Assessment (LCIA) tries to make a bridge between the traditional environmentally oriented and generic life cycle assessment (LCA) and the more site- and time-specific sustainability assessment (SA), which takes into account all three generally accepted pillars of sustainability: economic, social and environmental. This publication shows how all three techniques - which all share similar methodological frameworks and aims - can be combined to make the move towards an overarching LCSA possible. Conclusion LCSA has significant potential to be used by enterprises, governments, agencies for international cooperation and other organizations in society (such as consumers’ associations) in their efforts to produce and consume more sustainable Still more research and applications are needed, but its application is already feasible and encouraged to speed the learning curve of the society.

Challenges in implementing Life Cycle Sustainability Assessment (LCSA) and in an LCSA-based decision-making

K. P. Bzolilova-Kisheva, S. I. Olsen Technical University of Denmark, Lyngby, Denmark Life Cycle Sustainability Assessment (LCIA) has been proposed to be a combination of three assessments: environmental, economic and social (incl. socio-economic). In this way LCSA tries to make a bridge between the traditionally environmentally oriented and generic life cycle assessment (LCA) and the more site- and time-specific sustainability assessment (SA), which takes into account all three generally accepted pillars of sustainability: economic, social and environmental. In the process of trying to bridge and to draw from the strong characteristics of SA and LCSA, LCA encounters its own challenges.

Sustainability and human labour: how can LCA answer? B. Bugiani, D. Pansaniuk, E. Benetto Public Research Centre Henri Tudor (CRPHT), Esch-sur-alzette, Luxembourg In LCA the intrinsic dependence of productions on human labour (HL) is usually disregarded, without providing any clear argument. Apparently, HL is not considered to be related to and affected by, changes to the functional unit. Nevertheless, HL could be seen as the common numeraire among the three pillars of sustainability: environment, economic and social. This research aims at investigating the relationship between HL and LCA and at developing an operational framework to include HL in LCA. We defined three HL types (qualified worker, technician, manual worker). A comparative LCIA of the HL types was carried out using an environmentally extended input-output model of EU-27. Afterwards, ten agri-food and industrial LCAs case studies were modified for hybrid LCAs, adding HL inputs to existing LCIs. The LCIA comparison showed that a qualified worker always generates impacts greater than other workers. The impact of average HL is higher in EU countries with the highest household expenditures’ budget. Within the case studies, the HL significantly contributes to the total impact for several categories (e.g. fossil and ozone depletion up to 16% and 20%, respectively). We argue that an eco-profile of HL should always be added to LCI models that entail a significant direct human contribution: adding inputs of HL to the LCI of a product or process can improve its accuracy. This could enable to establish a common framework (same LCI) to account for HL under the three pillars of the life cycle sustainability assessment. So far, additional cost and social/organizational data of HL might be integrated in LCIs to provide useful information and an added value for more comprehensive assessment of the real life cycle cost (e.g. through addition of salaries and wages to the Life Cycle Costing (LCC) analysis) or social quality factors of labour (e.g. through implementation of further labour impact categories in the Social Life Cycle Assessment - SLCA) in a production chain. The proposed methodology can be used for a future implementation of HL at a level of unit process in LCA. By using a hybrid approach, possible double counting with non-human (i.e. machine driven) labour is easily avoided. However, humans are not machineries and they are driven by flows of information, knowledge, educational and cultural experience, and so forth. These are essential items for our sustainable development but how to integrate them into human labour LCI profiles remains an open task.

What life cycle sustainability assessment does and does not for new and innovative technologies P. Mason1, O. Amerighi1, F. Buttol1, A. Zamagni1, 3Enea, Bologna, Italy 2Enea Research & Study Unit, Rome, Italy Performing a sustainability assessment of new and innovative technology is a complex task, as showed by the definition itself, which refers to two big issues: Technologies

SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting
Evaluating multiple dimensions of sustainability in the case of bioenergy production based on multi-criteria analysis and life cycle assessment

Per capita individual options are evaluated compared to a kind of “Business-As-Usual” (BAU) reference scenario until year 2050. This BAU scenario assumes a moderate and steady barriers in the implementation of effective GHG reduction strategies evaluated options together with their ranking depending on subjective weighting profiles in a transparent way can facilitate decision processes and help in understanding can lack individual acceptance, or can be associated with high investment costs as a major obstacle to their implementation. Showing the advantages and disadvantages of the different results compared to the most frequently used purely economic perspective. While specific measures are very attractive from an economic long-term perspective, they

Reducing the carbon footprint of the Swiss energy system: which options are most sustainable?

A. H. Pandya-Wargo, H. Oosda, K. Nagata

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Fast growing mega cities in developing Asian countries are faced with municipal solid waste management (MSWM) related problems due to rapid urbanization, industrialization and population growth. Proper waste management with energy and material recovery prolongs the life of existing landfills, contributes in providing renewable energy and reduces pollution.

Although the need of shifting from landfilling to more environmentally sound solutions of solid waste management system is obvious, developing Asian countries have their own way of thinking, lifestyle, culture, budget related issues and concerns that reflect on the social and economic priorities in their decision making. For example, the fact that many scavengers lives depend on collecting and reselling plastic waste from the landfill to private recycling plants may interfere with the calorific value requirement of an incineration plant.

This study attempts to take into account the social and economic related considerations in Life Cycle Assessment (LCA) by using an integrated, survey based methodology called Environmental Load Point (ELP) developed in Nagata laboratory of Waseda University. ELP has broadened indicators categorized in 9 impact categories, which are energy depletion, global warming, ozone layer depletion, acid precipitation, resource consumption, air pollution, ocean and water pollution, waste disposal, and ecosystem influence. The results are weighted with national factors from the national newspapers to find out the importance of each impact categories in the concerned country. Additionally, Life Cycle Cost (LCC) is combined with ELP results to give cost estimation of the constructed scenarios. This combination is called Best Available System (BAS) for MSWM. ELP represents the social considerations while LCC represents the economic factor of sustainability.

Different results are constructed in this study with different portion of waste being recycled and incinerated, considering the composition of local waste and number of employed scavengers, in the way that a decision maker may help to determine how the Swiss result may help to improve the quality of the job market as well as taking a better MSWM technology with higher confidence because it has incorporated the ecology, economy, and social concerns. Moreover, text mining result is a reflection of the national concerns and priorities, thus it increases agreeability among the related community.

Towards comparative life cycle sustainability assessment of road marking systems

M. M. Muehlbach, A. Klein, K. G. Groenke

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Public purchase decisions are made at the expense of shrinking budgets at one hand and increasing demand for environmentally friendly goods on the other. This study looks at both economic and environmental impacts of road marking considerations using the whole life cycle from manufacturing to disposal. For the first time all four major binder-based raw material options are evaluated that can be considered to equip a road section with road markings that provide high visibility even at wet nights for a period of ten years. For the latter part of this study an external expert panel has reviewed the assessed scenarios. Social aspects are considered in a second step. It is not trivial to quantity these.

Evaluating multiple dimensions of sustainability in the case of bioenergy production based on multi-criteria analysis and life cycle assessment

P. J. Lesken

Finnish Environment Institute, Joensuu, Finland

Environmental impacts of products and services have been traditionally the main focus in life cycle assessment (LCA). Recently, other dimensions of sustainability including economic, social and even cultural aspects have been received more and more attention in addition to ecological impacts. Multi-criteria analysis (MCA) is a toolbox of methods that evaluate the properties of decision alternatives with respect to multiple, usually conflicting decision criteria. First, this presentation discusses how MCA can be utilized in LCA when evaluating the sustainability of products and services. The most important benefits of MCA are connected to integration of impact assessments not measured directly in commensurable units and incorporation of subjective preferences into the assessment framework. In general, the performance of decision alternatives depends on the weights given to various decision elements of the decision hierarchy and the performance of the decision alternatives with respect to the lowest level elements. Different life cycle stages capture the life cycle of the production alternatives from raw material and utilization to end use. This second presentation demonstrate the empirical results of forest biomass based bioenergy production in recent Finland that was the topic of recent research project funded by the Agency of Technology and Innovation. The project carried out the comparison of the alternative production chains in the methodological framework described above. The analyzed production chains were as follows: (a) Local heat entrepreneurship based on forest chips (Eco energy cooperative). (b) Wood pellets produced in Finland and distributed to domestic and global markets (Ilomantsi pellet plant). (c) Direct peat combustion in large combined heat and power (CHP) plants (Forment CHP, Joesuu; (d) Biofuels produced from both forest biomass and peat (Varkaus experimental plant). The empirical results of the multi-dimensional comparison of the production chains including economic, environmental, social and cultural sustainability as well as the overall performance when all dimensions are taken into account simultaneously are presented. In addition, the methodological gaps and future developments needed are discussed.

Reducing the carbon footprint of the Swiss energy system: which options are most sustainable?

C. Bauer, P. Ecke, K. Volkart

Paul Scherrer Institut, Villigen psi, Switzerland

One of the main objectives of the research project CARMA (Carbon Management in power generation) is the comparative evaluation of potential options for the reduction of Greenhouse Gas (GHG) emissions from the energy system in Switzerland within the framework of future energy scenarios. This assessment is carried out by applying Multi-Criteria Decision Analysis (MCA) methodology. The MCA approach allows considering a comprehensive set of performance indicators addressing environmental, economic and social aspects in decision making and therefore taking into account all three pillars of sustainability; besides these objective criteria, it also allows considering subjective stakeholder preferences, which are used for weighting of the indicators. These preferences are established by a purpose built interactive web interface. The combination and aggregation of performance indicators and preference profiles results in a single performance index for each mitigation option, which can be used for a ranking of these alternatives.

The evaluated GHG reduction options cover the most important economic sectors in terms of GHG emissions: the residential sector, traffic, power generation, and industry. The indicators are compared to a kind of “Business-As-Usual” (BAU) reference scenario until year 2050. This BAU scenario assumes a moderate and steady economic growth as well as a slightly increasing population in Switzerland going along with an increase in passenger and freight transport as well as the habitable surface area per capita. Depending on the indicator weighting profile used for the MCA - i.e. on the subjective preferences - the comprehensive evaluation of GHG reduction options can lead to different results compared to the most frequently used purely economic perspective. While specific measures are very attractive from an economic long-term perspective, they can lack individual acceptance, or can be associated with high investment costs as a major obstacle to their implementation. Showing the advantages and disadvantages of the evaluated options together with their ranking depending on subjective weighting profiles in a transparent way can facilitate decision processes and help in understanding barriers in the implementation of effective GHG reduction strategies.

Evaluating of sustainability as Environmental performance of the regional energy systems

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One of the main objectives of the research project CARMA (Carbon Management in power generation) is the comparative evaluation of potential options for the reduction of Greenhouse Gas (GHG) emissions from the energy system in Switzerland within the framework of future energy scenarios. This assessment is carried out by applying Multi-Criteria Decision Analysis (MCA) methodology. The MCA approach allows considering a comprehensive set of performance indicators addressing environmental, economic and social aspects in decision making and therefore taking into account all three pillars of sustainability; besides these objective criteria, it also allows considering subjective stakeholder preferences, which are used for weighting of the indicators. These preferences are established by a purpose built interactive web interface. The combination and aggregation of performance indicators and preference profiles results in a single performance index for each mitigation option, which can be used for a ranking of these alternatives.

The evaluated GHG reduction options cover the most important economic sectors in terms of GHG emissions: the residential sector, traffic, power generation, and industry. The indicators are compared to a kind of “Business-As-Usual” (BAU) reference scenario until year 2050. This BAU scenario assumes a moderate and steady economic growth as well as a slightly increasing population in Switzerland going along with an increase in passenger and freight transport as well as the habitable surface area per capita. Depending on the indicator weighting profile used for the MCA - i.e. on the subjective preferences - the comprehensive evaluation of GHG reduction options can lead to different results compared to the most frequently used purely economic perspective. While specific measures are very attractive from an economic long-term perspective, they can lack individual acceptance, or can be associated with high investment costs as a major obstacle to their implementation. Showing the advantages and disadvantages of the evaluated options together with their ranking depending on subjective weighting profiles in a transparent way can facilitate decision processes and help in understanding barriers in the implementation of effective GHG reduction strategies.

Evaluating of sustainability as Environmental performance of the regional energy systems

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LC02B-4 Integrating life cycle analysis, human health and financial risk assessment for the evaluation of contaminated site remediation

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When evaluating remediation technologies for contaminated soil and groundwater, the beneficial effect of the remediation, namely cleaner soil and groundwater, are mostly emphasized without consideration of the environmental and social impact of the remediation activities themselves. Nevertheless, practitioners and decision makers can rely on a broad range of decision tools that can help them to achieve a better balance between economic, social and environmental health aspects of contaminated land remediation. A holistic approach for the management of contaminated land should ideally include an assessment of the environmental risk of the contamination, an assessment of the environmental, social and health impact of the remediation process and a cost-benefit analysis of the remediation project.

A life cycle framework, including a life cycle management (LCM) approach structuring environmental activities and life cycle analysis (LCA) for a quantitative estimation, can be helpful for the selection of site remediation options with minimum impact on the ecosystem and human health. Besides addressing the environmental impact of the remediation activities, attention should also be paid to the consequence of reintroducing a remediated site into the economy.

Moreover, certain soil remediation technologies, especially the more ‘gentle’ remediation technologies are characterized with a lot of uncertainty with regard to the time frame in which the final remediation goals will be achieved. Unexpected situations can result in an increase of the costs of the remediation project. Therefore, there is a need for practical tools that help practitioners in choosing the correct technology that will not only be effective but also will minimize the financial risk associated with the cleanup.

In the present study, several methods that can be used to estimate the environmental, financial and health impact of a soil remediation process were compared. The case studies worked out in this paper want to provide a basis for a more soundly selected soil remediation technologies based on human health, environmental impact and financial risk criteria.

LC02B-5 Developments in Social Life Cycle Assessment (S-LCA) for Life Cycle Sustainability Assessment (LCSA) - application to the construction and demolition sector in France

A.L. Ross
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The results of a project aiming at developing a methodology for sustainability analysis dedicated to infrastructures and buildings construction projects will be presented. This research project was carried out in collaboration with ADEME (French agency of environment and energy control), University of technology of Troyes, the Industrial Ecology Club (guild) of Aube and Eiffage (French public works firm). The project is based on a specific case-study concerning the construction of a part of the ring road of Troyes city (Aube, France) where alternative construction materials and techniques, such as secondary raw materials and local natural resources, have been used. A sustainability LCA framework was designed, built on environmental and social LCA methodologies to assess the environmental and social efficiency of such construction projects.

It was applied to the case study to compare its global performance with a similar case which would have been conducted in “business as usual” conditions. An environmental LCA was considered in two cases: (a) existing international standards and (b) alternative construction techniques. At the same time, a S-LCA methodology was developed on the basis of UNEP-SETAC Guidelines and applied to the French sector of building and construction, to assess social impacts supported by the system’s stakeholders. Results showed a high contribution of natural mineral resources use in the total environmental impact, due to extraction and transportation. It was also demonstrated that the energy necessary for asphalt production was much higher than the one for its implementation. Environmental impacts are thus highly dependent on asphalt production and natural mineral resources’ quantities and origin. Regarding social impacts, specific impacts categories, indicators and data were searched for and an impacts screening was conducted. Based on sectorial data, it focuses on two stakeholders’ categories: workers and local communities. Final results highlight the fact that S-LCA needs strong methodological developments to address intra Europe comparative case studies and to produce methodologies for system definition, data inventory, impacts characterization, reference databases and specific indicators.

LC02B-6 Life cycle costing of farm milk production - cost assessment of environmental impact mitigation strategies

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The objective of the project was to quantify the costs of one of the production chains of milk in the French sector: the French sector of Building and Construction, to assess social impacts supported by the system’s stakeholders. Results showed a high contribution of natural mineral resources use in the total environmental impact, due to extraction and transportation. It was also demonstrated that the energy necessary for asphalt production was much higher than the one for its implementation. Environmental impacts are thus highly dependent on asphalt production and natural mineral resources’ quantities and origin. Social impacts, specific impacts categories, indicators and data were searched for and an impacts screening was conducted. Based on sectorial data, it focuses on two stakeholders’ categories: workers and local communities. Final results highlight the fact that S-LCA needs strong methodological developments to address intra Europe comparative case studies and to produce methodologies for system definition, data inventory, impacts characterization, reference databases and specific indicators.

LC03 - Increasing scientific and policy understanding through meta-analysis of life cycle assessments

LC03-I Clarifying estimates of life cycle greenhouse gas emissions from electricity generation technologies: the LCA harmonization project

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Thousands of LCAs of electricity generation technologies have been published. Quality of these studies has varied considerably, as have reported estimates of life cycle GHG emissions. We have completed a systematic review of the literature that included: exhaustive identification and collection of English language LCAs of electricity generation technologies with a no-blanket publication type (journal article, report, conference paper, thesis); and, multiple, independent reviews of each candidate reference by an interdisciplinary review team that met regularly to ensure consistent screening based on quality of LCA methods, completeness of reporting and modern relevance of evaluated technology.

Results:

- Estimates varied mainly owing to differences in assumptions of key parameters. It is possible to adjust previously published LCA results to use more commensurate input assumptions and system boundaries.
- We have quantified the global breakdown of the different processes as assessed both in terms of greenhouse gas footprint and production costs Change in GHG impacts and costs are assessed in parralel. Discussion on sources of revenues (GHG, water use, land use) with a measure of the financial costs or benefits of production changes.

Conclusion:

This study couples environmental impacts and costs, providing a general approach to improve the environmental footprint of milk production on a large range of impacts (GHG, water use, land use) with a measure of the financial costs or benefits of production changes.

LC03-2 Meta-analysis of life cycle analysis studies on electricity generation with carbon capture and storage

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3Currently, electricitity generation contributes to 40% of global carbon dioxide (CO2) emissions. Carbon capture and storage (CCS) technology is widely recognized as an
appropriate option to achieve ambitious CO2 reduction targets. In the last decade, numerous life cycle assessments (LCA) on environmental impacts of electricity generation with CCS have been conducted. This meta-analysis comprises fifteen LCAs of the three CCS technology routes (post-combustion, oxyfuel, pre-combustion) for greenhouse gas reduction for different regions (Europe, United States, Japan, global), different fuels (hard coal, lignite, natural gas), and different time horizons (between present and 2050). The meta-analysis provided a better understanding of the impacts and identified the key parameters that have significant effects on the outcomes. The study addresses three key questions: 1) Is LCA an appropriate method to evaluate the environmental effects of CCS, and with what validity or limitations?; 2) Is it possible to draw general conclusions regarding the environmental performance of CCS power plants compared to power plants without CCS from the existing LCAs?; 3) Do certain trends arise across the different capture routes or fuels used?

A first methodology to generate simplified models for WT environmental performances has been designed (reported in the special issue of the Journal of Industrial Ecology) and is now improved with a better identification of the GHG variability assessment. Variability of GHG performances of onshore wind turbines, generated for a representative sample, is assessed through the running of Monte-Carlo simulations to identify the key parameters having the biggest influence on the results. Based on these Monte-Carlo simulations, we plotted GHG performances distributions for two key identified parameters: the WT life time and the annual average wind speed. A set of generic GHG performances curves has been defined as a function of these key parameters. Results are ranging from 2.7 to 119.7 gCO2eq/kWh, a range which is comparable to the mentioned IPCC literature review. These results can be adjusted as a function of either one or both key parameters. This methodology will be applied later for simplified life cycle approaches.

LC03-3

Simplified life cycle approach: GHG variability assessment for onshore wind electricity based on Monte-Carlo simulations

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The environmental impacts of electricity production systems have been widely assessed over the past years with many published LCAs in the literature. In the special case of greenhouses gases (GHG) from wind power electricity, the LCA results variability observed is very high, for example ranging from 2 to 81 g CO2eq/kWh in a literature review performed by the IPCC in 2011. Such result might lead policy makers to consider LCA as an inconsolable method. For environmental impacts from electricity generation this is a sensitive issue.

There is a need for a more comprehensive approach to assess the GHG variability so as to define generic results which meet a general consensus. Different attempts have been initiated in order to address this problematic, the use of meta-analyses in LCA being one of them.

The main objective of this paper is to build a representative model of onshore wind turbines (WT) to assess environmental performances with a simplified life cycle approach. A first methodology to generate simplified models for WT environmental performances has been designed (reported in the special issue of the Journal of Industrial Ecology) and is now improved with a better identification of the GHG variability assessment. Variability of GHG performances of onshore wind turbines, generated for a representative sample, is assessed through the running of Monte-Carlo simulations to identify the key parameters having the biggest influence on the results. Based on these Monte-Carlo simulations, we plotted GHG performances distributions for two key identified parameters: the WT life time and the annual average wind speed. A set of generic GHG performances curves has been defined as a function of these key parameters. Results are ranging from 2.7 to 119.7 gCO2eq/kWh, a range which is comparable to the mentioned IPCC literature review. These results can be adjusted as a function of either one or both key parameters. This methodology will be applied later for simplified life cycle approaches.

LC03-4

What can meta-regression analysis tell us about variations in life cycle assessment (LCA) results for greenhouse gas (GHG) emissions estimated for advanced biofuels?

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This paper presents a systematic literature review of LCA studies of advanced biofuels (i.e. biomass-based fuels produced from lignocellulosic materials and microalgae).

The study, notably econometric LCA studies, now provides an overview and estimated using a meta-regression analysis in order to clarify conclusions about their environmental performances. LCA has been widely applied to calculate the Global Warming Potential (GWP is an impact indicator for GHG emissions) associated with biofuel life cycle. Those LCA results can vary significantly depending on various factors: assumptions at biomass production step (N2O emission estimations, inclusion of direct and indirect Land Use Change-LUC), the type of computer analyzed, such as low-power light desktop, or high-power workstation, may dominate the total impact; future studies should therefore base their estimates on a large sample to smooth out this variation, or explicitly restrict the analysis to a specific type of computer.

Estimates of manufacturing impacts, especially those related to printed circuit boards and integrated circuits, are highly uncertain and variable; such uncertainties have a significant impact on the results: 1) power plant efficiency and energy penalty of the capture process, 2) CO2 capture efficiency and purity, and 3) fuel origin and composition. However, the normalization indicates only a small impact from CCS power plants on total global environmental impacts.

The meta-analysis proves that LCA is a helpful tool to investigate the environmental consequences associated with CCS. Differences in the underlying assumptions of the LCAs and limitations in the data available are the principal reasons for the uncertainties. More systematic research is needed to reduce these uncertainties. The type of computer analyzed, such as low-power light desktop, or high-power workstation, may dominate the total impact; future studies should therefore base their estimates on a large sample to smooth out this variation, or explicitly restrict the analysis to a specific type of computer.

This abstract is based on a paper currently in press with the Journal of Industrial Ecology, due to be published in early 2012 in a special issue on meta-analyses of life cycle assessment.

LC04-1

Quantification of uncertainty and spatial variability of characterisation factors in the new global LCIA method IMPACT World+

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IMPACT World+, a new LCIA method representing an update of the IMPACT 2002+ LCIA method, was developed as a regionalised methodology covering the entire global scale, and including uncertainty information encompassing spatial variability and model uncertainty. Up to now uncertainties were only quantified in life cycle inventory databases. IMPACT World+ now provides quantitative uncertainty estimates for each characterisation factor (CF) and thus allows for a complete uncertainty analysis for an entire LCA study. This presentation introduces the approaches used to estimate, quantify, and combine uncertainty and spatial variability for CFs in each impact category. The uncertainty and spatial variability are quantified and kept separately, allowing for differences in spatial variability of CFs in different spatial scales. This is necessary for water use impacts, and urban/rural archetypes for Respiratory impacts, or soil and water archetypes for metal toxic impacts compared to a global or continental average CF. This results in two semi-quantitative pedigree-matrices, per impact category respectively representing uncertainty and variability. Assigning a GSD2 to each of the five uncertainty/variability classes ranging from “no” to “very high” uncertainty/variability allows translating the quantitative into qualitative information. The resulting GSD2 values for the identified main coefficients that compose the CF, e.g. for human health if, dose-response, and severity factor, can then be combined into a total GSD2 for each CF. A pragmatic and operational solution was required to provide estimates for characterisation factors that count from a handful in some impact categories such as Eutrophication up to thousands for human health or ecotoxicity. IMPACT World+ is the first LCIA method to provide...
quantitative uncertainty for each CF using an estimation framework that is consistent with life cycle inventory uncertainty estimates from e.g. ecoinvent. Given the various types and sources of uncertainty contributing to the overall uncertainty of a CF, the estimates provided are not covering all uncertainty sources and types, and might have a somewhat limited accuracy. They are however an important operational starting point to consistently apply uncertainty analysis in LCA, ultimately allowing to quantify the confidence in LCA results and hence the related conclusions and decisions.

LCA0A-2

Quantification of uncertainty of characterisation factors due to spatial variability

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Except for a minority of foreground production sites, elementary flow geographic location is only known to the country resolution. More precision is needed to pick the right regionalized characterisation factors (s-CF) from a set. Countries are usually covered by several s-CF, and their value might span several orders of magnitude. So far, this source of variability has not been quantified. This paper presents a general method quantifying the uncertainty created by the dichotomy in spatial resolution between inventory and impact assessment.

For each country, a generic CF (g-CF) has to be calculated with the s-CF covering it. Two elements are necessary to build the g-CF: the probability density function (PDF) of each s-CF, and a set of weighting factors. The weighting set provides a likelihood of emission on the zone covered by each s-CF, an information lacking in the generic unit process. The average and standard deviation of the g-CF is not calculated directly from the weighted s-CF. Instead, the PDF of the g-CF is built by adding the weighted PDF of each s-CF. The average value of the g-CF can be calculated from the PDF and used in deterministic calculations. The standard deviation could be useful if the resulting PDF can be approximated by a normal or lognormal. Otherwise, the full PDF should be reported and used directly in a Monte Carlo simulation.

Finally, the probability (CV = average variation of the g-CF) of the CV of the generic unit process for the g-CF will be higher, and this augmentation of uncertainty reflects the spatial variability that cannot be taken into account, due to the lack of spatial information in the generic unit process.

The impact category chosen to demonstrate this methodology is water use on human health. The spatial delineation of this method is the intersection of countries and water basins, resulting in 808 cells. The likelihood of water use in each cell is based on data from the Watergap model. China is covered by 20 watersheds. The corresponding 20 s-CF are lognormally distributed with CV between 0.6071 and 0.6218. After adding their weighted PDFs, the resulting g-CF is bimodal, with a CV of 7.63. This means that if a good quality water source occurs somewhere in China, without further information on the watershed of consumption, it will be characterized with a g-CF of a value potentially much more for higher than lower the right s-CF, and roughly 10 times more uncertain.

LCA0A-3

Matrix-based sensitivity and uncertainty assessment for evaluating human intake of pesticide residues in food

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Multiple pathways contribute to human exposure towards pesticides: inhalation after air emissions, ingestion after soil and water emissions and, most importantly, ingestion of directly treated food products. For the latter, we developed a dynamic multicropl model for assessing pesticide residues in food crops and subsequent human intake. However, full uncertainty analysis is still lacking. We already identified half-lives in plants and time between substance application and crop harvest playing a crucial role, but other aspects may also be important.

We designed a simple but accurate regression model with time from application to harvest, half-life in plants, residence times in the environment and key substance properties as input variables. Additional information are identified by analyzing several input variables, therefore setting weights on parameters in a regression framework. We studied the uncertainty propagation of the model output applying a new approach of calculating the overall output uncertainty as a function of the matrix of relative sensitivities of input variables and the covariance matrix expressing their correlations. Model output, i.e. human intake fractions from consumption of food crops treated with pesticides, showed highest relative sensitivities across substances to half-lives in plants and on plant surfaces as well as to the time between substance application and crop harvest. Total output sensitivity is a function of the crop species and is highest for leafy vegetables (lettuce) and fruit trees (apple). We also studied the variability across pesticides, from which we derive crop-specific regression models predicting residues in food crops across pesticides within a factor of 10 of those calculated with the complex model as a function of only a handful of input variables. These simplified models are adequate to assess direct residues for multimedia models used for risk and impact assessment and, hence, enable the user to calculate direct pesticide residues only providing a very limited set of input information.

LCA0A-4

Uncertainty classification and implementation in life cycle impact assessment: application to freshwater ecotoxicity of pesticide application to maize in The Netherlands

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How to deal with uncertainty has become a key challenge for integrated assessments. As yet, the application of an uncertainty analysis is not common practice in life cycle assessments. A proper analysis will be facilitated when it is clear which types of uncertainties exist. The aim of this research is to set up a framework to classify levels of uncertainty in life cycle impact assessment (LCIA) and demonstrate the practicability of the framework with a case study example on freshwater ecotoxicity caused by pesticide application in The Netherlands.

Three levels of uncertainty were distinguished. (i) Statistical uncertainty, arising from measurement errors, analytical imprecision, and limited sample size; (ii) Decision rule uncertainty, caused by ambiguity or controversy about how to quantify or compare social objectives; (iii) Model uncertainty, defined as uncertainty about the relations and mechanisms being studied. To quantify statistical uncertainty, uncertainty distributions need to be derived for input parameters and propagated to output uncertainties, e.g. via Monte Carlo simulation. Decision rule uncertainty and model uncertainty can both be made operational with the help of a choice analysis.

A case study that addresses the application of pesticides to maize in the Netherlands was performed to show the application of the various uncertainties for freshwater ecotoxicity. Sensitivity in freshwater ecotoxicity damage scores was quantified by performing a Monte Carlo analysis with chemical-specific input parameters set as uncertain. Decision rule uncertainty was determined by identifying choices in the damage quantification, i.e. availability of toxicity data, choice of effect factor model (linear or non-linear), and the damage factor (modeling up to midpoint or to endpoint). Model uncertainty was quantified by including and excluding pesticide transformation products.

Results showed that damage can vary substantially depending on the value choices made. Parameter uncertainty can increase to a large extent when a more accurate model is applied. Going from midpoint to endpoint applying an uncertain damage factor decreases the damage slightly, but hardly changes uncertainty. Only when transformation products are included, going from midpoint to endpoint increases median damage clearly.

LCA0A-5

Data quality metrics in Life Cycle Impact Assessment: application to a case study of cellulosic biofuel

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Although guidelines exist for assessing data quality in life cycle impact assessment (e.g., ISO-14044), they are seldom implemented satisfactorily in practice. A need therefore exists for transparent, clear methods for data quality metrics that facilitate the prioritization of data needs and enhance the reliability of LCIA. Monte Carlo (MC) methods, such as sensitivity and uncertainty analysis are used to identify the most influential inputs and to understand how input uncertainty (variability and lack of knowledge) is propagated through to the calculation of output metrics. However, MC methods are rarely applied in LCIA. Here we demonstrate the application of sensitivity analyses coupled with a data quality evaluation scheme, to assess uncertainty in output metrics in our LCA "Carbon Tool", which quantifies the environmental and human health impacts associated with national-scale cellulosic biofuel production. Program outputs include CO2, O2 and CO2 emissions, and life cycle carbon footprint. Output metrics are input variables and are integrated in the model through the carbon stock in crops, production stage and transport phase. The uncertainty of data quality metrics is calculated using the Spearman rank correlation coefficient to identify influential variables for each output metric, with specific application to the carbon mass balance. We then evaluate the uncertainty in influential system variables, using a qualitative data quality evaluation scheme coupled with Monte Carlo simulations. The most influential factor is the carbon stock in crops, which is determined by the carbon content in crop biomass, and is based on assumptions (medium rating for data acquisition). For human health impacts, specifically those for PM emissions, the three most influential system variables are the residence time in the environment and key substance properties.
Developments in life cycle assessment (LCA) have led to new life cycle thinking applications such as the macro LCA approach (M-LCA), an extension of consequential LCA (C-LCA) that implements elements of prospective LCA in order to model medium- or long-term environmental impacts related to global economic perturbations caused by major changes occurring in multiple life cycles. In M-LCA, economic impacts are based on the GTAP model, an economic general equilibrium model (GEM), which provides various production functions for each economic sector in each region of the world in response to a given economic change. The environmental impacts of each regional economic sector are then computed according to the LCA methodology. As uncertainty related to GEMs and LCAs is recognized as significant, the uncertainty associated with M-LCA is evaluated. To that end, an uncertainty analysis was conducted on an M-LCA comparison of two European Union (EU) energy policies (business as usual vs. bioenergy). Uncertain exogenous variables and internal parameters used by GTAP were combined in order to develop 27 scenarios that were run in GTAP to define a tree of potential economic consequences caused by each EU policy under the assumption of each scenario. Environmental impact uncertainty for the 27 scenarios was then assessed using a Monte-Carlo (MC) analysis. Results of the uncertainty analysis show how the M-LCA comparison of EU policies is not negligibly affected by uncertainty for climate change and natural resource scarcity since the comparison is more uncertain for human health and ecosystems. The uncertainty analysis also highlights that several sources of uncertainty in M-LCA cannot be assessed due to lack of information on data uncertainty (external data used for the linkage of GTAP and LCA databases and forecasts used to model the evolution of temporal variables) and the difficulty in comparing GTAP results with historic data. Additionally, it appears MC analysis is not adequate to study uncertainty propagation in complex models such as M-LCA. Indeed, due to the significant quantity of uncertain parameters, the time required to conduct the MC simulations makes this approach impossible besides the extensive computational resources. Therefore, the development of another approach based on an uncertainty management method more suitable for large models, like Gaussian quadrature or Fourier transformations, would improve the management of uncertainty in M-LCA.

LCOB-1
Technological, geographical, time-related uncertainty measurements for textile spinning and weaving processes
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Life Cycle Assessment (LCA) is very dependent on the quality, relevance and reliability of the Life Cycle Inventory (LCI) data sets selected by the LCA-practitioner. When modeling a system, the representativeness of the LCI data set is complemented by the appropriateness of the data set in the context of the specific system. The appropriateness characteristics, in how far a data set in a system model represents the truly required process of product. According to the ICLC handbook [1], the use of not fully appropriate data is justifiable only if this is not relevantly changing the overall LCIA results compared to using fully representative data; otherwise the lower achieved representativeness shall be documented in the report. But when the required data is missing the practitioner has limited possibilities to evaluate any differences between the required data and the available data.

This paper aims at evaluating the appropriateness of different LCA-practitioner choices regarding the geographical, technological and time related representativeness in the modeling of a product life cycle. The examples are taken from two technologies from the same industry domain that behave differently and require different LCA methodologies.

First, different LCI data sets for spinning and weaving processes in the textile industry are inventoried. The precision, completeness, representativeness and methodological consistency of these LCI-data sets are characterized by the used inputs, the data sources and the representativeness in terms of geographical, technological, and time-related context. The most appropriate data set is defined for each process, and the relevance of using the other data sets is illustrated.

Second, the methodology to assess the appropriateness of the selected LCI data set is presented. A simple example is given for the case of LCI data set for spinning processes, which shows that the representativeness of the selected LCI data set can be quantified. The approach is then applied to the case of weaving processes, which shows that the representativeness of the selected LCI data set can be assessed in a similar way.

Finally, the appropriateness of different LCI-data sets for spinning and weaving processes is assessed. The results show that the selected LCI-data sets for spinning processes are more appropriate than the selected LCI-data sets for weaving processes. This is because the selected LCI-data sets for spinning processes are more consistent with the geographical, technological, and time-related context of the processes.
Interpretation of the results is crucial and a specific uncertainty analysis method has been developed. Uncertainty is analyzed separately for Physical Input (PI) data and Emission Factors (EF). The pedigree matrix takes into account reliability, completeness, temporal, geographical and technological representativeness of data according to five different quality levels. Accuracy is increased by introducing a specific factor for the availability of Physical Input primary data versus secondary. Finally Emission Factor quality are specific of industrial activity. The uncertainty factors are used together to evaluate the global uncertainty.

The majority of the carbon footprint (85%) calculations are in the “good” level, while 10% are of “middle” uncertainty and finally 5% are evaluated as “very good”. When making a decision, it is important to allocate budget toward the most important topics. This uncertainty approach enables decision-makers to choose under the best conditions. The EDF framework can be considered in decisions, helping us to evaluate and improve the inventory each year. All uncertainty factors are based on regional expert judgment and should be challenged by external expert (eg. Quality of background LCIs database).

Implementing Carbon Footprinting is an important step towards an Environmental Footprint management by introducing the life cycle perspective and involving the whole company. Nevertheless such a wide perimeter implies a complex calculation protocol and the uncertainty calculation will have a huge importance to tackle the complexity of this management and implement the best decisions.

Finally, the authors stress that even if uncertainties exit, these shall not be a barrier for taking action.

LCOMB-5 Uncertainty and variability in the carbon footprint of U.S. coal-fired power production M. Hauck1, Z. Steinmann1, I.J. Laurenzi2, R. Karuppiah2, A. Faldi2, M.A.J. Huijbregts1

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The overall carbon footprint of power generation can be calculated using life cycle assessment (LCA). For most LCAs, average conditions are used to estimate the environmental impacts of a process or product. However, regional and technological differences in production methods, use, and disposal can cause specific life cycle impact (e.g. GHG emissions) to be lower or higher than that of an “average” life cycle. Moreover, uncertainty in process data used to model life cycle stages may affect the accuracy and precision of life cycle impact assessments. Whereas uncertainty is defined as lack of knowledge and can potentially be reduced by additional research, variability is an inherent characteristic of supply chains and the environment and cannot be reduced. The aim of this study is to quantify the contributions of uncertainty and variability to the range of the carbon footprint associated with coal-fired electricity production in the US. Two qualitative factors of spatial and temporal variability upon the life cycle emissions and the power plants they supply and power plant efficiency. We also characterized parameter uncertainty, e.g. the methane emission associated with a coal basin. The LCA included three stages: mining, transport and power generation, and utilized a functional unit of 1 kWh of electricity generated at the plant. Parameter uncertainty was quantified via Monte Carlo simulation, whereas variability was taken into account via the efficiencies of power plants and coal transportation reports by the U.S. EIA. We present two different carbon footprints for U.S. power plants with uncertainty ranges. Our results show that the variability in electricity plant efficiencies particularly lead to a large overall variance of the life cycle emissions of coal power. Results indicate that improvements in inventory data and assessment parameterization reduce the variance of the life cycle emissions. The results can be used to assist decision-makers in ranking the carbon footprints of coal plants and facilitate the comparison of coal power emissions with other power generating technologies on a statistical basis.

LCOMB-6 A protocol for approaching uncertainties in life-cycle inventories Monte Carlo analysis - a practical example using aquaculture feeds J. Hentriksson, J.B. Guinée, R. Heijungs, R. Kleijn, G.R. de Snoo

CML Leiden University, Leiden, Nederland

Although LCI values often are presented in absolute numbers, uncertainty and variability are common traits of both foreground and background data. Uncertainties result from limited temporal, spatial and technological coverage of both economic and environmental flows, with a direct influence on results. In LCIs of food production systems, however, the influence of variability (ontological uncertainty) may be increasingly predominant as production is governed by natural fluctuations (e.g. yields). Outcomes of LCA results describing the same production system may therefore vary with up to an order of magnitude. Aquaculture feeds are here used as a practical example to demonstrate the proposed approach to uncertainties in LCIs. The modelling includes foreground data collected from feed mills in Asia and literature sources, while background data derive from the ecoinvent v 2.2 database. Each processes within the system boundary was approached using a standard protocol to assign mean, standard deviation and distribution to most economic and environmental flows. Each of these variables were based either on primary data, weighted averages derived from a meta-analysis or a numerical unit spread assessment (NUSAP) pedgree. The inventories were later simulated using a Monte Carlo analysis to generate confidence intervals for individual flows. Using relevant up-to-date inventories is crucial for achieving accurate results and taking uncertainty into account is the only way to justify these results. We, therefore, herein present a practical way on how to consistently source and analyse inventory data using a mix of real values, weighted averages and NUSAP estimations. This allows for a wide range of data sourcing and a constructive strategy for highlighting areas of great uncertainty and identifying data gaps.

LC05 - Monetisation for weighting and aggregation in Life Cycle Assessment and Cost-Benefit-Assessment

LC05-1 Development of national average weighting factors in LIME2 - Visualization of the variability of external cost using statistical analysis N.I. Isburo1, M.S. Sakagami1, K.K. Kuriyama1, A.I. Isabu2

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Recently several methods of economic evaluation have been published in the scientific literature increasing the credibility and the review process. Examples of more recent methods are based on monetary valuation of endpoints (Isburo et al., 2004; Weidema, 2009), the Ecotox method based on a monetary valuation of midpoints (Finnveden et al., 2006), and panel methods for midpoints (Soares et al., 2006; Huppes et al., 2007). Methodological aspects of weighting methods are also reviewed and discussed in detail (Miettinen and Hopfens, 2005). The results are not only easy to understand but can also be used for cost-benefit analysis. While the best way to allocate economic values to environmental impacts such as a loss of health or a decline in biodiversity is still in the development stage and has not yet been fully established. This study summarized a result of development of national average weighting factors with visualizing of the variability of external cost using statistical analysis. Conjoint analysis was applied to weight across several safeguard subjects and random parameter logit model was adopted to measure the confidence interval of external cost.

LC05-2 Environmental damage cost factors per functional unit of transport activities, heat & electricity generation in Germany P. Preiss, W. Müller, J. Roos, V. Will, S. Torras Ortu, A. Kuhn, J. Reumann-Schichtenberg, R. Friedrich

Universität Stuttgart, Stuttgart, Germany

For decision support, results of LCA often are weighed to be weighted aggregation of impacts and evaluation or ranking of alternatives. Impacts can be expressed in monetary terms to facilitate appropriate taxing or subsidies, and cost-benefit-analysis, etc. If impacts on human health and the environment are expressed in monetary terms they are called environmental economic costs (EEC). The share which is not internalised into economic decisions is called external costs. Starting in the 1995, with the External Costs of Energy (ECE) project-series methods for estimating EDC have been developed. The methodology has been further improved in several EU-projects. In 2011, within a project for the German Federal Environmental Agency, cost factors have been re-calculated for different transport activities, heat & electricity supply in Germany including operation and up- and downstream processes, also outside Germany. A large amount of results is available providing differentiation between energy carriers and technologies for heat and electricity. Moreover, with regard to transport activities different energy carriers, modes and different technologies have been assessed. Results are available at www.ExternE.info. The updated and extended impact pathway approach provides results which are more reliable and conclusive as it combines site specific assessments, as far as possible, but also includes average values for different source characteristics and regions. The uncertainties due to spatial variability inherent in many LCA methodologies are transparent because country specific values are further differentiated into sub-regions, urban and rural environment, and different heights of releases. The results can be used to support decision making, perform cost-benefit-analysis and test more simplified approaches in the future.
Innovation to develop new packaging systems with reduced environmental impacts

Recently, an improved land use method has been developed with the UNEP/SETAC Life Cycle Initiative project (LULCIA, 2008-2011). This method relates land use to six new indicators: biotic production (BPP), erosion regulation (ERP), fresh water regulation (FWRP), mechanical and physicochemical water purification (WPP) and carbon sequestration (CSP). The other regulation services values are estimated through current compensation costs, as they are considered essential (conservative approach). As a local impact category by nature, spatial variability and the availability of the compensation systems are taken into account. Economic valuation assumptions will be discussed.

Finally, this method brings a new level of interpretation and potentially allows LCA to assess other impacts related to land use, such as aesthetics and recreational aspects. This method will be applied on a case study involving the comparison of production locations for bio-based polyesters.

The developed monetisation factors for non-renewable resource consumption consist hence in using trend market prices multiplied by a factor correcting for the excessive productivity loss and carbon tax. The other regulation services values are estimated through current compensation costs, as they are considered essential (conservative approach).

The methodology approach developed is based on the following analysis:

- The market price is driven away from the optimal price since, however, an independent peer-review process according to ISO 14040 & 14044 will still be required. To simplify the LCIA methodology, the PI was applied on two existing treatment plants managed by Suez Environnement in France. The plant comparison using the PI calculated with ReCiPe is not conclusive, since the confidence interval of the difference of the average PI values is zero (too high uncertainties). The same evaluation with monetized scores, augmented by operational costs, gives a clear preference for one of the two sites. Further research is ongoing to add infrastructures data in the LCIA calculations and to implement LCA uncertainties into the performance index.

**LC05-4**

Development of an integrated indicator for land use based on ecosystem services

First, an independent peer-review process according to ISO 14040 & 14044 will still be required. To simplify the LCIA methodology, the PI was applied on two existing treatment plants managed by Suez Environnement in France. The plant comparison using the PI calculated with ReCiPe is not conclusive, since the confidence interval of the difference of the average PI values is zero (too high uncertainties). The same evaluation with monetized scores, augmented by operational costs, gives a clear preference for one of the two sites. Further research is ongoing to add infrastructures data in the LCIA calculations and to implement LCA uncertainties into the performance index.

**LC05-5**

How to correct price for monetising non-renewable resource consumption?

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**LC05-6**

Life cycle management (LCM): Success factors and barriers

**LC06-1**

Barriers and success factors in the use of LCA and ecodesign tools at Nestlé

Nestlé, the World's leading Nutrition, Health and Wellness Company, is committed to environmentally sustainable business practices. We assess the environmental impacts of our products using LCA and ecodesign tools. While LCA has been shown to be useful for claims and communication of the performance of our products to third parties and the public, the timeline and cost of conventional LCA is not practical for a widespread application throughout the company.

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**LC06-2**

Mainstreaming life cycle management: using a sector based and regional approach in Northern France in the textile, seafood, packaging and mechanical sectors

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3. Université de Montréal, France
4. CIRSEE - Suez Environnement, Le pecq, France
5. INNASA Toulouse, LBF, Toulouse, France
6. Nestlé Research Center, Lausanne, Switzerland
7. Intertek RDC, Brussels, Belgium
8. European Commission
9. De Caevel, S. Standaert, E. Van Overbeke
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SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting 111
MAUD competitiveness cluster, Villeneuve d’Ascq, France

CETIM, Marécal-en-Barœul, France

Aquibou, Boulougne sur mer, France

UP tex, Marécal-en-Barœul, France

Whilst Life Cycle Management is becoming commonplace in larger corporations, or forward thinking governments, it is far from mainstream. To achieve sustainable production and consumption patterns, LCM needs to be taken up by whole supply chains that include many small and medium enterprises. These businesses typically lack the financial capacity or human resources to implement LCT tools on their own, and are wary of working with support organisations outside of their sector or local area.

In Northern France, the textile, seafood, packaging and mechanical sectors are developing strategic action plans to integrate Life Cycle Approaches (including ecosdesign and product environmental labelling) into businesses, education and research organisations. Each study is led by a competitiveness clusters or technical centre working within the sector.

The paper will present the results of the benchmark of life cycle initiatives and tools relevant to each sector, and assessment of the existing capacity of businesses, education bodies and research centres in the region. Focus will be given to how potential actions are prioritised through engagement with key stakeholders (such as businesses, universities and professional federations) and how this inclusive process maximises with success factors and helps overcome barriers to implementation.

The four action plans are developed in parallel, enabling the sectors to identify cross cutting actions. The paper will explain how this process is managed through a network of “Life Cycle Champions”. Champions have been trained in the eight sectors, and meet regularly to exchange experiences in implementing life cycle approaches and identify cross cutting projects. The 4 other sectors will undertake the strategic action planning process in a second “wave”, to incorporate learnings from the first process.

This innovative approach to mainstreaming LCM leverages sectoral and regional networks to help overcome barriers to implementation. From a business perspective, integration with existing professional organisations means that SMEs access advice and tools through organisations that they already know and trust. Working with several sectors in parallel through the Life Cycle Champion network encourages a multidisciplinary approach, essential to improving decision making across entire supply chains.

**LC03-6 Driving proactively the sustainability agenda for the European detergents and maintenance products industry, via the A.I.S.E. Charter for Sustainable Cleaning**

V.S. Sejourne1, D.W. Walker2, S.N. Nissen1

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A.I.S.E., the International Association for Soaps, Detergents and Maintenance Products, has a long tradition of proactive work towards sustainable production and consumption. Its main overall scheme is the A.I.S.E. Charter for Sustainable Cleaning, encouraging the adoption of sustainability management practices at all stages of the product life cycle; launched in 2004 in all EU countries plus Norway, Iceland and Switzerland, the Charter covers all products categories of the detergent, cleaning and maintenance products’ industry.

Participating companies report regularly progress on Key Performance Indicators, leading to the publication of an annual sustainability report. As a new approach to the Charter is a success with 160 companies committed, covering approximately 85% of the total industry’s production output; An update of the Charter has been rolled out in 2010, introducing a product dimension to the existing Charter requirements. This fits very well with the overall objectives of the European Commission SCP/SIP Action Plan, and particularly the Ecodesign Directive.

**LC04-6 Life Cycle Assessment, from an evaluation tool to a collaborative eco-design enabler for electric vehicles**

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1RENAULT / MINES PARISTECH, Guyancourt, France

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The automotive industry is facing major challenges and the problem is strong in order to reduce production cost and usage value within the capacity of the nature to support the mobility growth.

This goal will be achievable only when a co-innovative product design will be set up, involving the whole value chain [1]. This is an ambitious target and this paper will show how life cycle assessment evaluation tool could be a major contributor to bring the various parties altogether.

Several example are identified, from the more obvious which is the critical review during which the practitioner will open his work to Research Institutes / Universities or Environmental Non-governmental Organizations. Regarding the impact assessment, reliability can be worked with Research Institutes when comprehension can be studied with Customers. Concerning Inventories employees and suppliers will work hand in hand and finally for the scope definition, this will be a good opportunity to involve the customers in order to define the relevant functional unit. This last point is particularity true when speaking of the electric vehicle, a new technology and potentially a major change in people habits of buying and consuming their mobility.

One method is the definition of the functional unit for electric vehicles LCA [4]. The main difficulty [5] is to define a function equivalent between thermal and electric vehicles. The ILCD handbook [2] recommends a functional unit defined by four items: What, How much, How long and in What way. The reason for any doubt take place in the last item, in what way. This question was studied under two approaches, one “product centric” based on functional analysis and one “people centric” based on customer (emotional) needs. Then we can enlighten the main differences between the thermal vehicle strength - reaurance and aesthetic - versus electric vehicles ones - environmental friendly and fun. Therefore, equivalent functional units shall add a reassurance dimension to the electric vehicle functional unit such as an easy access to a “long autonomy range” vehicle when needed.

This experience on the electric vehicle shows also that LCA can be a very useful tool to bring the stakeholders (unusual ones as NGOs as well) around the table with a positive and constructive scientific approach.

**LC05-6 LCT in the floor-covering industry: the strategy of Tarkett**

M. Guisoni1, E.L.L.K Bezart2, E.N.R.L. Bemot1, A.C. Ayed2

1Public Research Centre Henri Tudor, Luxembourg- kirchberg, Luxembourg

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Tarkett is world-wide leader in innovative flooring and sports surface products, providing integrated solutions to professionals and end-users. Despite its long time concern about environmental issues, actions remained not harmonized so far. The main tool reflecting environmental performances of Tarkett activities and products was the regular publication of five environmental “Key Performance Indicators” on global production. The need for a comprehensive sustainable development strategy to be integrated in the daily practice has emerged and Tarkett is now engaged with a multifold challenge. To tackle this endeavor, Tarkett has chosen the support of the Public Research Centre Henri Tudor. Life-Cycle Thinking (LCT) has been identified as main approach, since the products are at the core of the environmental strategy system. Tarkett deals with a wide range of products spread over 30 worldwide production sites. It families of products, and therefore a wide range of materials, the implementation of LCA as a fact based practice for process and product environmental improvement has therefore become a priority. Although LCA is used as an eco-design driver and a strategic tool, the company is aware that this tool is not sufficient at its actual level of development to address some specific issues. Therefore Tarkett is engaged in complementary development studies and processes. The adopted approach is a progressive integration of LCA as a decision-making tool in a coherent way for all Tarkett’s branches. First Tarkett company is aware that this tool is not sufficient at its actual level of development to address some specific issues. Therefore Tarkett is engaged in complementary development studies and processes. The adopted approach is a progressive integration of LCA as a decision-making tool in a coherent way for all Tarkett’s branches. Further development phase is now launched; the vision is to combine the complementary tools already used by Tarkett in the LCT process, in order to set a robust decision making based on eco-innovation criteria.

**LC06-6 Promoting use of life cycle management in Finnish companies - challenges, benefits and suggestions for future value networks**

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Life cycle thinking (LCT) and life cycle assessment (LCA) along with other life cycle (LC) methods are important tools in assessing environmental impacts of products and services, and to support environmental decision making in companies. Use of those methods can also help companies to find business opportunities by taking precautionary actions. This study presents the main drivers and barriers for companies to apply LCT, LCA and other LC methods. We also suggest a roadmap for the promotion of these methods in companies and their value networks. We first assessed the methodological challenges of the LCT, LCA and other LC methods from the company point of view. The minority of those tools was assessed in several case studies. The assessments were based on the data from literature and companies. Several stakeholder workshops were organized to get practical views on the use of LC methods. The current and future use of LC methods in companies was also studied using an internet questionnaire and thematic interviews. They revealed that the companies can coarsely be categorised in four main company types regarding their knowledge, resources and potential to utilize life cycle methods in practice. The findings were supported by the case studies. Three company types were named as ‘interested outsiders’, ‘learners’ and ‘forerunners’. Additionally a large group of companies are not aware of the use of life cycle methods and their potential benefits. The main drivers for the environmental management of companies included legislation requirements, improvement of cost-efficiency and customer requirements, among others. A large number of...
companies are not familiar with life cycle methods and their potential benefits. Additionally, especially of small and medium-sized enterprises (SMEs), often have no temporal, and economic resources to learn and educate themselves on the benefits of using LCT and LCA. The main challenge related to wide use of LCT and LC methods in companies is probably related to the communication problem between the LC researchers and companies, and therefore must more practical approach need to be used when spreading LCT in wide scale. The next step in promoting the use of LCT and LC methods in decision making in practice will be a pilot project, in which all the actors within a region, value-chain or sector will be introduced to work with each other in a networking process, including specific type of training for SMEs.

LC07 - The UNEP-SETAC Life Cycle Initiative: a decade of supporting the global LCA community

LC07-1
Scientific legacy of the UNEP-SETAC Life Cycle Initiative: contributions and significance
B.W. Vignon1, G. Sonnenmann2, S. Valdivia3, J. Fava4
1SETAC, Pensacola, United States of America
2United Nations Environment Programme, Paris, France
3Five Winds, West chester, United States of America
The UNEP-SETAC Life Cycle Initiative is a joint venture formed in 2002, among several purposes, to foster the development, validation, and dissemination of methods, tools and practices for life cycle assessment and management. Over its ten year history the Initiative has conducted dozens of projects which have contributed to the efficiency, effectiveness, and rigor of life cycle approaches on a global scale. This presentation will address those contributions from the viewpoint of meeting critical needs for maintaining and enhancing the quality of the science underpinning life cycle approaches. It will also place those developments in the context of emerging research and practice from academic, government and business organizations, providing a perspective on the significance of the Initiative’s contributions to the science of LCA.

LC07-2
Top 10 points about life cycle every government decision maker should know
A.L. Quirolo1, S.V. Valdivia2, G. Sonnenmann3
1ECO GLOBAL S.A., San jose, Costa Rica
The 10 bullets that government officials should remember about Life Cycle Approaches when considering sustainability decisions is a contribution of the UNEP/SETAC Life Cycle Initiative to the discussions for the next UN World Summit for Sustainable Development.

LC07-3
Strategizing capacity development for life cycle management - cases from Vietnam and Malaysia
A. Wangel
Technical University of Denmark, Kgs. lynby, Denmark

LC07-4
Water use in life cycle assessment and water footprinting: outputs and prospects of the working group WULCA
S. Pfister1, A.M. Boulay2, A. Koehler3, E. Aoustin4
1UC Santa Barbara / ETH Zurich, Zurich, Switzerland
2CIRAIG, Montreal, Canada
3PE International, Office Switzerland, Winterthur, Switzerland
4Veolia Environnement, Paris, France

LC07-5
Establishing knowledge and data resources, facilitating communication and training, providing limited support for application, and creating international networks for spreading LCT in wide scale

LC07-6
Future action points are the harmonization of existing LCIA methods and inventories

LC07-7
Meanwhile, life cycle assessment and water footprinting: outputs and prospects of the working group WULCA

LC07-8
The UNEP-SETAC Life Cycle Initiative: a decade of supporting the global LCA community
been of lower priorities so far, however, with increasing demand for both robust water use information and related impact assessment, the supply of representative water use data it becomes a relevant issue, especially due to the high spatial variability of water use and related impacts.

LC07-5
Value of a Life Cycle approach in evaluating the environmental impacts of packaging for food and beverage applications
L.F. Flanagan1, J.F. Fava2, B.V. Vignon3, S.V. Valdivia4
1PE International & Five Winds Strategic Consulting, Westchester, United States of America
2SETAC, Pensacola, United States of America
3UNEP, Paris, France
An articulation of the benefits of the life cycle approach to design, manufacturing, use and end of life management of packaging for food applications is important to further examination of the role of packaging within the nexus between security and safety of packaging in food and beverages and environmental protection. Key items of focus for the research and analysis included, but not limited to:
- What is the value of a life cycle approach for beverage and food products and packaging?
- What is the value of including all life cycle stages in evaluating the packaging/food systems to reduce overall life cycle impacts?
- What is the value of including multiple impacts in evaluating the packaging/food systems to reduce overall life cycle impacts?
- What is the value of manipulating the food and/or beverage into an evaluation of the packaging life cycle impacts?
- What characteristics of future LCA studies should be considered when evaluating the food/packaging life cycle?
Examples of how the waste management hierarchy and LCA results interface/connect
This presentation will present the results of study to evaluate the Value of a Life Cycle Approach in Evaluating the Environmental Impacts of Packaging for Food and Beverage Applications.

RA01 - Applying models to risk assessments: from the organism to the ecosystem level

RA01-1
What do over-fish effects on individual endpoints translate to at the population level?
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In the model, individuals are assumed to sense and avoid contaminated habitat with a certain probability, which depends on contamination level: avoidance of toxicant influences the feeding behaviour of the organisms, this in turn affects all the other biological processes. Model rules and parameters are based on data from the literature; for toxicity, only data from standard laboratory tests (survival, reproduction and avoidance) are used. The model has been parameterized and evaluated using Pattern Oriented Modelling (POM): in POM, models are required to simultaneously reproduce a diverse set of patterns. The model has been run with two simulation scenarios where polluted area and concentrations of toxicant (CaSO4) are the same, but spatial arrangement and connections between clear patches are different. In both cases the presence of patches of suitable habitat allows the population to grow, although the size is reduced with respect to the control. At the lowest concentration, the organisms cannot sense the toxicant and therefore do not avoid the contaminated areas: for this reason toxic effects are much less than proportional to the concentration. From the comparison of the two scenarios, it appears also that when the population is more affected during the spring peak, it is then more resistant during the fall peak, and vice versa.

RA01-2
Exploring the consequences of spatial heterogeneity in pesticide exposure using an individual-based model of collembolan populations
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Suitable habitat for soil organisms may be scarce, thus leading to locally high population densities, because soil, being more static than water or air, is heterogeneous; physical conditions often vary widely on a scale of a few centimetres. Moreover, toxic chemicals are likely to be unevenly distributed in the soil as well. To explore the consequences of these heterogeneities for the population dynamics of soil invertebrates, we developed a spatially explicit individual-based model of the collembolan Folsomia candida. In the model, individuals are assumed to sense and avoid contaminated habitat with a certain probability, which depends on contamination level: avoidance of toxicant influences the feeding behaviour of the organisms, this in turn affects all the other biological processes. Model rules and parameters are based on data from the literature; for toxicity, only data from standard laboratory tests (survival, reproduction and avoidance) are used. The model has been parameterized and evaluated using Pattern Oriented Modelling (POM): in POM, models are required to simultaneously reproduce a diverse set of patterns. The model has been run with two simulation scenarios where polluted area and concentrations of toxicant (CaSO4) are the same, but spatial arrangement and connections between clear patches are different. In both cases the presence of patches of suitable habitat allows the population to grow, although the size is reduced with respect to the control. At the lowest concentration, the organisms cannot sense the toxicant and therefore do not avoid the contaminated areas: for this reason toxic effects are much less than proportional to the concentration. From the comparison of the two scenarios, it appears also that when the population is more affected during the spring peak, it is then more resistant during the fall peak, and vice versa.

To conclude, a combination of spatial heterogeneity and stressors can lead to unexpected effects of toxicants at the population level. Individual-based models help disentangle and understand these effects and therefore add ecological realism to environmental risk assessment of chemicals.

RA01-3
A comparison of deterministic and stochastic matrix population models to evaluate ecological risk of chemicals
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Environmental management decisions regarding toxic chemicals are mainly based on measurements on individuals, e.g., mortality and fertility. However, the aim of environmental management is, most often, to protect populations, not individuals. The necessary extrapolation from individuals to populations introduces a large degree of uncertainty in the risk assessment process. Presently, this uncertainty is dealt with by using fixed safety factors that are set to be protective in the majority of the cases. One method to reduce this uncertainty may be to use population models. However, before such models can be used routinely in ecological risk assessment of chemicals, the types of models to use must be determined as well as the level of model complexity necessary to provide an accurate risk assessment for different management scenarios. The objective of the present study was to determine whether simple deterministic matrix population models can be used as a first tier in risk assessment of a chemical, or if more complex models that include environmental stochasticity are needed. Matrix population models for two species of fish (eel and perch) were used in combination with dose--response data for a metal mixture, 2,3,7,8-tetrachlorodibenzo-p-dioxin, and tributyltin. From the deterministic models, the maximum acceptable exposure was determined as the level where the population growth rate (λ) is equal to one, which means that the population size is stable. For the stochastic model, the 5th percentile for λ=1 was used, which means that there is 5% probability for population decline. The results were compared to traditional risk ratios, based on individual level responses, and safety factors (in accordance with European Union guidance documents). Although the results of the stochastic models are more informative with regards to probability for adverse ecological effects, the results of the deterministic models clearly reduced uncertainty compared to the traditional risk ratios. This means that simple deterministic models, in combination with appropriate safety factors, can reduce the risk for over- as well as underprotective risk assessments.

RA01-4
Stochastic density dependent matrix model to extrapolate effects of toxicants from laboratory tests to population-level effects: case study on Folsomia candida exposed to cadmium
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This ecosystem model was developed with a focus on EE2-endpoints reliable for risk assessment and will be validated with data from other whole-ecosystem studies performed at the Experimental Lake Area (ELA, Ontario, Canada): (i) two years of reference data (ii) three years of exposure to environmentally-relevant concentrations of the synthetic hormone 17-ethinylestradiol (EE2) and (iii) five years of recovery data. EE2 was chosen because it is a key estrogenic compound measured in effluents from industrial plants and wastewater treatment facilities worldwide. Two ecological endpoints were measured: reproduction of three-spined stickleback and survival of common club-tail dragonflies. Endocrine disruption has been measured in many aquatic environments across the world but the consequences on the whole ecosystem are still unclear. Experimental approaches for characterizing the ecological impact of such disturbances are costly and time-consuming. Therefore, ecological models are currently being developed to support risk assessors in their decisions. Ecosystem models are required for assessing effects at high levels of organization, but the need for extensive calibration for a specific ecosystem limits their application in ecological risk assessment. This study aims at providing risk managers with an ecosystem model able to predict critical changes in aquatic environments impacted by endocrine disrupters. The objective is to find a compromise between the data available and the complexity required for the model. The ecosystem model is developed with field data obtained from a multi-year whole-ecosystem study performed at the Experimental Lake Area (ELA, Ontario, Canada): (i) two years of reference data (ii) three years of exposure to environmentally-relevant concentrations of the synthetic hormone 17-ethinylestradiol (EE2) and (iii) five years of recovery data. EE2 was chosen because it is one of the most widespread and potent endocrine disrupters. Indeed, the fallfseau minnow population collapsed after the second year of EE2 additions and endocrine disruption was observed in the other fish species as well. The developed ecosystem model considers direct effects of EE2 on fish species but also the consequences on the whole ecosystem through ecological interactions (feeding, competition and predation). The model is based on simplified equations of the AQUATOX model (USEPA, 2002) with additional equations for endocrine disruption. Three fish classes are used (juveniles, females, and males) with a variable representing the reproductive ability associated with each class. The phytoplankton and zooplankton are modeled also as co-occurrences with matrix population models. Three fish classes are used (juveniles, females, and males) with a variable representing the reproductive ability associated with each class. The phytoplankton and zooplankton are modeled also as co-occurrences with matrix population models.

RA01-6

An ecosystem model for risk assessment of aquatic environments impacted by endocrine disrupters

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Endocrine disruption has been measured in many aquatic environments across the world but the consequences on the whole ecosystem are still unclear. Experimental approaches for characterizing the ecological impact of such disturbances are costly and time-consuming. Therefore, ecological models are currently being developed to support risk assessors in their decisions. Ecosystem models are required for assessing effects at high levels of organization, but the need for extensive calibration for a specific ecosystem limits their application in ecological risk assessment. This study aims at providing risk managers with an ecosystem model able to predict critical changes in aquatic environments impacted by endocrine disrupters. The objective is to find a compromise between the data available and the complexity required for the model. The ecosystem model is developed with field data obtained from a multi-year whole-ecosystem study performed at the Experimental Lake Area (ELA, Ontario, Canada): (i) two years of reference data (ii) three years of exposure to environmentally-relevant concentrations of the synthetic hormone 17-ethinylestradiol (EE2) and (iii) five years of recovery data. EE2 was chosen because it is one of the most widespread and potent endocrine disrupters. Indeed, the fallfseau minnow population collapsed after the second year of EE2 additions and endocrine disruption was observed in the other fish species as well. The developed ecosystem model considers direct effects of EE2 on fish species but also the consequences on the whole ecosystem through ecological interactions (feeding, competition and predation). The model is based on simplified equations of the AQUATOX model (USEPA, 2002) with additional equations for endocrine disruption. Three fish classes are used (juveniles, females, and males) with a variable representing the reproductive ability associated with each class. The phytoplankton and zooplankton are modeled also as co-occurrences with matrix population models. Three fish classes are used (juveniles, females, and males) with a variable representing the reproductive ability associated with each class. The phytoplankton and zooplankton are modeled also as co-occurrences with matrix population models.
The developed approach introduces a two-stage PBT classification scheme - primary classification of parent chemicals and secondary classification of stable degradants for ERA of pharmaceuticals based on FAHP and FI system as an objective and sensitive method in order to overcome uncertainties and compensate data gaps in literature. A new methodology for PBT prioritization of chemical inventories has been developed in view of regulatory requirements for quantitative assessment of persistence, bioaccumulation potential and toxicity of chemicals. CATALOG/OASIS and EPI Suite QSAR models for calculating P, B and T endpoints have been used. The methodology is implemented in a software system for computerized PBT classification of large chemical inventories. Two cyclic volatile methyl siloxanes, octamethylcyclotetrasiloxane (D4) and decamethylcyclopentasiloxane (D5), have recently been subjected to close scrutiny of their environmental fate and health effects. It is thus not surprising that difficulties were encountered when existing methodologies for exposure hazard assessment were applied to these chemicals. Here we introduce these difficulties with the aim of extracting the lessons that can be learned from these chemicals.

**RA01-D**

**A new methodology for PBT prioritization of chemical inventories**

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A new PBT prioritization methodology has been developed in view of regulatory requirements for quantitative assessment of persistence, bioaccumulation potential and toxicity of chemicals. CATALOG/OASIS and EPI Suite QSAR models for calculating P, B and T endpoints have been used. The methodology is implemented in a software system for computerized PBT classification of large chemical inventories. Comparative risk assessment of arsenic trioxide and its substitutes for occupational exposure in Murano (Venice, Italy) artistic glass production was explored.

**RA02-D**

**Comparative risk assessment of arsenic trioxide and its substitutes for occupational exposure in Murano (Venice, Italy) artistic glass production**

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Comparative risk assessment involves the assessment of the exposure of a chemical to humans or the environment in terms of risk components that are RL, RS and RP. FI method enables to use expert opinions instead of strict formalizations. Fuzzy inference (FI) systems are used for complex matrices that cannot be regulated or formulated. It is aimed to propose an approach to handling these matrices in order to evaluate the magnitude of these effects. RP hierarchy contains the sources of the pharmaceuticals and factors related with treatibility indicating the possibility of release to the environment. RS hierarchy deals with persistence and union operations using fuzzy membership functions. FAHP and FI method enables to use expert opinions instead of ampic formulations which is beneficial for the complex assessments that are affected by numerous factors and cannot be completely formulated like ERA. Proposed approach reduces uncertainties and subjectivities and provides more rigid RM that can be used as a guide for the risk management attributes.

**RA03-D**

**Exposure hazard assessment: lessons learned from cyclic volatile methyl siloxanes**

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Two cyclic volatile methyl siloxanes, octamethylcyclotetrasiloxane (D4) and decamethylcyclopentasiloxane (D5), have recently been subjected to close scrutiny of their environmental fate and health effects. It is thus not surprising that difficulties were encountered when existing methodologies for exposure hazard assessment were applied to these chemicals. Here we introduce these difficulties with the aim of extracting the lessons that can be learned from these chemicals.
RA03-2

Environmental monitoring data: support for an effectiveness assessment and a success control under REACH

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Environmental specimen banks support competent authorities in the assessment of chemicals. Together with national and EU-wide monitoring systems they can give information for the identification of new substances of regulatory concern. Beyond the assessment of individual chemicals, monitoring data can also be used to develop indicators to evaluate the implementation of different chemical regulations by providing information on the impact of chemicals to human health and other compartments of the environment.

By end of 2012, the European Commission has to present a first evaluation of the effectiveness of the REACH regulation. Human biomonitoring and environmental monitoring programmes may provide valuable data to underpin this evaluation. In the EU there is a variety of environmental monitoring activities which have been established for various reasons. They are - in different degrees - suitable to indicate the implementation of REACH. A research project - funded by the German Environment Protection Agency (UBA) - analyzed the available monitoring programs (including environmental specimen banks) to identify those who can contribute to evaluate the effectiveness and the success of different REACH task, starting from specific tasks related to specific parts of REACH (e.g. registration) up to tasks related to the effectiveness evaluation of REACH as a whole.

In order to determine appropriate indicators and methods to evaluate the impact of the European chemicals legislation REACH, a detailed and complete review on ongoing environmental monitoring activities has been conducted. Furthermore, a guidance document for the use of environmental monitoring data with a view to the evaluation of chemicals has been developed and presented. It includes both the company’s self-monitoring as well as governmental monitoring and important regulatory focal points under REACH. Exemplary case sheets on selected chemicals were documented for the monitoring / identification of substances of concern, thereby using the Environmental Specimen Bank (ESB).

Future challenges in regulatory risk assessment go beyond time trends of individual substances. Effectiveness assessments of such regulations as REACH require indicators for the total environmental burden due to the wide dispersive uses of a large number of substances - and its effect on biodiversity. Environmental specimen banks can support such assessments and the elaboration of adequate indicators.

RA03-3

Mercury stable isotopes in seabird eggs from the NIST Marine Environmental Specimen Bank reflect a gradient from terrestrial geogenic to oceanic mercury reservoirs

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Environmental Quality Standards (EQS) for Persistent Organic Pollutants (POPs), the plan for integrated pollution prevention and control (IPPC) [3] and thus, ongoing environmental monitoring occurs in many Baltic countries.

Hexachlorobenzene, a fungicide which is no longer used in the EU, was below the EQS of 10 pg/kg in all fish analysed. Eels had higher concentrations with a median of 1.8 and a maximum of 183 pg/kg compared to 0.9 and 4.5 pg/kg in product.

Mercury concentrations in seabird eggs, as an indicator of the environment, have recently increased due to the global increase in mercury emissions, especially from coal-fired power plants.

The Fish Archive grows it will become possible to determine temporal and spatial trends of these and other substances.
and C8 (0.318 - 79.0 ng/g), perfluorooctanesulfonamidoacetates (N-MeFOSAA (<0.0031 - 8.11 ng/g), N-EtFOSAA (0.0058 - 9.00 ng/g), FOSAA (<0.0011 - 8.25 ng/g)), and perfluoropolyethers (PFPEs): C8 (0.176 - 31.7 ng/g), C9 (0.020 - 2.70 ng/g), C10 (0.020 - 0.880 ng/g), C11 (0.003 - 0.555 ng/g) were detected in over 80% of the samples. The long-chain PFCA s (C12 (0.0017 - 0.565 ng/g) and C14 (0.0017 - 0.049 ng/g) PFCA s), however, were only detected in 20% of the samples. Temporal trends can be observed for some of the analytes: PFOS concentrations peaked in 1986 (~ 30 ng/g) and reached a plateau before they began to decrease starting in the year 2000 (~ 4 ng/g) in Münster samples. A similar decline in PFOS concentrations (1999-2005) was also observed for samples from Halle. The temporal trend observed here for human PFOS contamination mirrors industrial production patterns, with the post-2000 decline in PFOS sera concentrations occurring concurrently with the phase-out of PFOS and relaxed chemical standards starting in 2000. A total of 320 samples were analyzed for DiPAPs and SAmPAP, although quantifications had been done only for 6:2/6:2 and 8:2/8:2 DiPAPs and SAmPAPs. Further confirmation using matrix matched calibration curve and standard addition will be carried out for 4:2/4:2, 10:2/10:2, and SAmPAPs. The 6:2/6:2 (~0.00048 - 0.762 ng/g) and 8:2/8:2 (~0.0004 - 0.285 ng/g) DiPAPs were detected in 46% and 32% of the samples, respectively. No distinct was observed for 8:2/8:2 DiPAP, however, an increasing trend could be observed for 6:2/6:2 DiPAP after year 2000.

RA04-6

New challenges for environmental specimen bank applications - banking for marine mammal health research
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RA04-7

Midpoint and endpoint indicators for global terrestrial acidification: a dilemma for decision-making
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RA04-8

Life cycle assessment of biofuels for transportation: understanding the effects of scale
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RA04-9

Life cycle assessment of biofuels for transportation: understanding the effects of scale
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RA04-10

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RA04-11

Midpoint and endpoint indicators for global terrestrial acidification: a dilemma for decision-making
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RA04-12

Global life cycle impact assessment on marine eutrophication
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RA04-13

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RA04-14

Global life cycle impact assessment on marine eutrophication
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RA04-15

Global life cycle impact assessment on marine eutrophication
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SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting
Accounting for greenhouse-gas emissions in LCA from the degradation of chemicals in the environment

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Chemicals are released into the environment at their end of life. As they degrade, emissions of CO2 and other greenhouse gases (GHG) occur, which are often excluded from LCA studies. This work addresses this methodological gap by presenting a method to account for (GHG) emissions from degradation, namely carbon dioxide (CO2), methane (CH4) and nitrous oxide (N2O). In addition, carbon accounting rules for biogenic and fossil carbon are discussed and several options are presented that provide a consistent framework for LCA studies.

A Life Cycle Impact Assessment (LCIA) model is proposed to estimate the multimedia distribution and degradation of chemicals released to the environment. The environmental distribution, along with emission factors and assumptions for each compartment (air, water, soil, sediments) is used to calculate emissions of CO2, CH4 and N2O following initial release of the chemical to either the air, water or soil compartments. The method is described and applied to nine organic chemicals. GHG emissions resulting from the treatment of these nine chemicals are shown to be significant when compared with the corresponding cradle-to-gate emissions, particularly for those situations where there is no prior wastewater treatment. This work is important for the design of effective wastewater treatment plants and for the assessment of chemical emissions. Overall, the method presented enables the accounting of GHG emissions that are currently neglected in many LCA and carbon footprint studies. The model has been parameterized for a generic environmental scenario but it can be adapted for more specific conditions. The main limitation and source of uncertainty is the potential lack of chemical-specific data required to model environmental fate of a chemical. Also, the method uses generic assumptions and emission factors, that might not be appropriate to describe local conditions.

RA04A-5
Water footprint and life cycle assessment frameworks: synergies and hurdles

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Water footprinting has come a long way in the past 10 years, from simple water volume inventories, to scarcity assessment, to damage oriented LCIA modelling of several impact pathways up to endpoints. With this increase in methodological developments and applications, the scientific and industrial communities are now debating about the ultimate meaning(s) of a water footprint. This paper aims to evaluate the synergies and hurdles between the so far developed water footprint approaches, with the traditional LCIA midpoint-endpoint framework. We therefore propose to demystify: a) Standalone versus full life cycle assessment water footprint; b) Single indicator versus multiple indicators; c) Intra-compartment versus trans-compartment assessment and d) Water footprinting of the chemical to either the air, water or soil compartments. The method is described and applied to nine organic chemicals. GHG emissions resulting from the treatment of these nine chemicals are shown to be significant when compared with the corresponding cradle-to-gate emissions, particularly for those situations where there is no prior wastewater treatment. This work is important for the design of effective wastewater treatment plants and for the assessment of chemical emissions. Overall, the method presented enables the accounting of GHG emissions that are currently neglected in many LCA and carbon footprint studies. The model has been parameterized for a generic environmental scenario but it can be adapted for more specific conditions. The main limitation and source of uncertainty is the potential lack of chemical-specific data required to model environmental fate of a chemical. Also, the method uses generic assumptions and emission factors, that might not be appropriate to describe local conditions.

RA04A-6
Chemical footprint from point sources in Sweden

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This study has identified a method to quantify the chemical footprint from point sources with data from the E-PRTR (European Pollutant Release and Transfer Register) togheter with USEtox. USEtox is often used in Life Cycle Impact Assessment. There is an EU-wide model that a few years ago was saying that industrial facilities (e.g. industries) emitting over certain thresholds have to report to a register, E-PRTR, annually. The industrial facilities covers 65 economic activities within the following 9 industrial sectors: energy, production and processing of metals, mineral industry, chemical industry, waste and wastewater management, paper and wood production and processing, intensive livestock production and aquaculture, animal and vegetable products from the food and beverage sector, and other activities. Data is provided in the register for 91 polluting plants following the 7 groups: greenhouse gases, other gases, heavy metals, pesticides, chlorinated organic substances, other organic substances and inorganic substances. Data was collected from the EEA website, where all E-PRTR data is available for all EU27 countries. The emissions were listed by amount to water and air respectively.

A calculation on the impact is made using the USEtox method as implemented in SimaPro. The USEtox model is an environmental model for characterization of human and ecotoxicity impacts in Life Cycle Impact Assessment and for comparative assessment ranking of chemicals according to their inherent hazard characteristics. In this study the impacts human toxicity (cancer and non-cancer) and ecotoxicity are included. The calculations are performed in SimaPro. The results are given in CTU (comparative toxic units).

The results for the year 2008. Sweden has delivered emissions for 53 substances, some to air or water and some to both. The total emission to air is very much larger than the total emission to water. The expected results are: an aggregated measure of the toxicity from the sources included in E-PRTR, a calculation on contribution to toxicity by different emissions, consideration of information on each substance's contribution to toxicity, identification of the most important chemicals. For these the results are divided in contribution to human toxicity and to ecotoxicity. This study makes it possible to discuss how useful this method is to quantify the chemical footprint by using data from E-PRTR and the USEtox method.

RA04B-1
Probabilistic environmental hazard assessment of implementing green chemistry property design guidelines to reduce acute and chronic aquatic toxicity

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Water footprinting has come a long way in the past 10 years, from simple water volume inventories, to scarcity assessment, to damage oriented LCIA modelling of several impact pathways up to endpoints. With this increase in methodological developments and applications, the scientific and industrial communities are now debating about the ultimate meaning(s) of a water footprint. This paper aims to evaluate the synergies and hurdles between the so far developed water footprint approaches, with the traditional LCIA midpoint-endpoint framework. We therefore propose to demystify: a) Standalone versus full life cycle assessment water footprint; b) Single indicator versus multiple indicators; c) Intra-compartment versus trans-compartment assessment and d) Water footprinting of the chemical to either the air, water or soil compartments. The method is described and applied to nine organic chemicals. GHG emissions resulting from the treatment of these nine chemicals are shown to be significant when compared with the corresponding cradle-to-gate emissions, particularly for those situations where there is no prior wastewater treatment. This work is important for the design of effective wastewater treatment plants and for the assessment of chemical emissions. Overall, the method presented enables the accounting of GHG emissions that are currently neglected in many LCA and carbon footprint studies. The model has been parameterized for a generic environmental scenario but it can be adapted for more specific conditions. The main limitation and source of uncertainty is the potential lack of chemical-specific data required to model environmental fate of a chemical. Also, the method uses generic assumptions and emission factors, that might not be appropriate to describe local conditions.

RA04B-2
Biodiversity footprinting - quo vadis?

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Biodiversity loss, and its potential impacts on human welfare, are an increasing environmental concern, and should be assessed in product assessments, in order to provide a more complete life cycle assessment. The aim of this paper is to present a method to account for biodiversity impacts in LCA. The two methods presented, in this paper, are the Food Footprint Methodology (FFM) and the Water Footprint Assessment (WFA). The FFM is a method to quantify the contribution to biodiversity of a product or activity, while the WFA is a method to quantify the contribution to human and ecosystem quality and resources. The WFA profile, can be further disaggregated putting in perspective the relative contribution of each impact pathway to the overall impacts on the water resource within each area of protection.
adequate support to decision-makers. Likewise, there is an upcoming trend to quantify environmental impacts of products in terms of so-called footprints, which should address biodiversity effects in addition to the conventional carbon and water footprints. However, biodiversity is a multifaceted concept with strong variation in time and space, which makes it difficult to assess. Some current methods are based on the unit “potentially disappeared fraction of species” (PDF), but the scale (e.g. biodiversity loss at the local, regional or global scales) and choice of which species should be protected are not consistently defined across impact categories. Therefore, impacts to biodiversity at local, regional or global scales are often aggregated, leading to misinterpretations of LCA results. Here, we attempt to provide a framework to guide methodological choice.

Clarifying why we are concerned about biodiversity loss is the first step towards determining what we should be measuring. We distinguish between valuing biodiversity due to intrinsic value or due to its utility for mankind. For the first, enough primary habitat needs to be conserved and the human-modified landscapes need to be managed to assure the persistence of populations of species. The utility can be manifold and the concept of ecosystem services could serve as a starting point that helps to structure, classify, and measure different functions that ecosystems provide for humans. We also highlight value judgments involved in assessment frameworks, indicators and weighting schemes.

To assess cause-effect chains of biodiversity loss, multivariate models, meta-analysis of literature of cause-effects from field surveys, extrapolation of lab experiments or expert opinion can be used.

RA04B-3
Valuating ecosystem goods and services in LCA

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In LCA models, resource assessment is centered on the notion of scarcity: depletion is evaluated using a static perspective by comparing a resource’s rate of abstraction versus the available stock and its rate of regeneration, or by quantifying the marginal extraction cost. As a result, a limited number of resources (essentially fossil fuels and minerals) is investigated while other goods and services (EGS) are basically ignored, despite their crucial role. Dynamic accounting is a prerequisite to consistently embrace the actual pressure of human activity on rivers resources, their marginal rate of regeneration and the interdependency of their production patterns. Hence, ecological modelling can be a way to build a consistent and practical framework of characterization of EGS in LCA. The GUMBO model details the internal behaviour of the global natural system (geosphere) and its interactions with the anthroposphere; it is adjusted with key metrics measured during the 20th century to reflect global dynamics. The model delivers the economic values of human, social, built and natural capitals (i.e. EGS) according to user-defined scenarios for the societal mankind during the 21st century. The use of monetary units enables direct comparisons among ‘capitals’ and is a strong vector to communicating results. However, it drives to a utilitarian, end-user perception of use’ usefulness, disregarding the role of indirect EGS and the past natural ‘investment’ to this capital. Therefore, other metrics developed in the field of sustainability indicators may be tested, such as exergy. Acknowledging the current fruitful EGS accounting in LCA, the emergy framework provides a measure of the global-scale geobiosphere work on a common physical numerator (equivalent joules of solar energy, sej). We expect GUMBO to improve consistency in the emergy evaluation of global natural processes and resulting Unit Emergy (UEV) of EGS, which can be used to obtain complementary (physical) information to the (economic) characterization of EGSs in LCA. Although regionalization of this framework remains unclear, it is expected to be highly representative at global scale and open the road to a comprehensive, ecology-oriented perspective in the evaluation of the natural capital and its use by human systems. The aim of this presentation is to illustrate the methodological approach and its preliminary outcomes.

RA04B-4
Exergetic footprint as indicator to assess the environmental sustainability of processes

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Exergy analysis has two key attributes for being used as an environmental indicator: first, given that the environment is used as a reference state, exergy is a measure of any thermodynamic deviation with respect to its normal state; second, it allows comparisons between inflows and outflows, regardless they are mass or energy streams, using the same physical units (exergy) for their analysis.

Besides, the exergetic footprint (ExF) bears in mind the exergy that still remains in products and highlights the use of exergy as a convenient unit of measure and comparison. In this paper, the (ExF) was used as a resource/waste accounting indicator for the environmental assessment of a production process. The proposed methodology was applied to a wood-based particleboard production process from a factory located in Galicia (NW Spain). The study was proposed as a gate to gate analysis of the production process. The foreground Inventory data has been collected through on-site interviews and visits. The background inventory data are from the database ecoinvent v2.2.

The total exergy consumption for the particleboard manufacturing process was determined as the sum of each input category exergy plus the exergy content of wastes, reaching a value of 17.7 GJ per functional unit. Meanwhile, to determine the ExF the exergy that still remains in the produced particleboard was also considered, and a value of 3.5 GJ per functional unit was obtained for the scenarios built, CEx ranged from 17.76 to 15.73 GJ-m3-particleboard and the ExF from 3.69 to 1.66 GJ-m3, for 0 to 100% of recycled wood wastes employed.

The material resources, especially wood material, were the main contributors to CEx and ExF, as it had been identified by the ecological footprint in a previous work. The results suggest that a clear improvement in the sustainability of the process could be attained by increasing the feasibility of using different waste materials in the design of the particleboard.

RA04B-5
Thermodynamic resource indicators and footprint in LCA: a case study of titania in China

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LCA has standardized methods for assessing emission impacts but no comparable methods for the accounting or impact assessment of resource use. This study contributes to the existing research by offering a comprehensive comparison of different resource indicators, in particular those based on thermodynamics, and testing them in a case study of titania in China.

The system boundary for resource indicators and the case study is defined as a thermodynamic hierarchy at four levels: the natural environment (CEENE), and three have different backgrounds: abiotic resource depletion potential (ADP), environmental priority strategies (EPS), and eco-indicator 99 (EI99). The foreground Inventory data has been collected through on-site interviews and visits. The background inventory data are from the database ecoinvent v2.2.

Results show that the scores of resource indicators of the chloride route for titania system are lower than that of the sulphate route. The thermodynamic footprint of the former is consistent with previous studies, but this is not the case for the sulphate route. Moreover, the thermodynamic footprint of the chloride route is consistent with previous studies, but this is not the case for the sulphate route. The thermodynamic footprint of the chloride route is consistent with previous studies, but this is not the case for the sulphate route.

Thermodynamic footprint can provide guidance on how to calculate a Product Environmental Footprint (PEF) and an Organisation Environmental Footprint (OEF), as well as how to create product category or sector specific requirements for use in Product Footprint Category Rules (PFPCR) or Organisation Footprint Sectorial Rules (OFSR). Each requirement in the PEF and OEF guidelines has been chosen taking into consideration the recommendations of existing environmental accounting methods. Although existing methods align on some of the guidelines they provide, discrepancies and/or lack of clarity remain on a number of important decision points, which significantly reduces the consistency and comparability of the results. In some cases, it was necessary to go beyond the level of guidance provided in existing documents. An example is the coverage of impact categories and the models used for calculation.

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SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting
RA05 - Classification and risk assessment of metals and inorganic substances

RA05-1
Speciation in the transformation/dissolution examination of tungsten and antimony metal and compounds
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Speciation is held to be a key factor in the human health and environmental effects of metals and compounds. In this study, we present the results of the examination at pH 6 and 8.5 of the T/D (Transformation/Dissolution) characteristics of W (tungsten) metal and several of its compounds, measuring the concentrations of total dissolved W and the tungstate ion, WO₄²⁻. We have also determined the T/D behaviour of Sb (antimony) metal and several of its compounds with respect to total dissolved Sb, and for the 1 mg/L loadings, the speciation of dissolved Sb(III) and Sb(V). We show how the T/D data have been used to derive UN GHS (United Nations Globally Harmonized System of Hazard Classification) or EU CLP (Classification, Labelling and Packaging) outcomes. We used high performance liquid chromatography and inductively-coupled plasma mass spectrometry to analyse the corresponding dissolved species. For the W compounds examined, the T/D data revealed that all dissolved W existed as WO₂⁻. Na₂WO₄, 2H₂O ammonium para- and meta-tungstate were readily and completely soluble, yielding measured W concentrations of about 67 mg/L, and WO₄²⁻, concentrations in the total elemental analysis of 1.0 mg/L, loadings, which correspond to all W dissolved as WO₂⁻. Compared to an acute ERV (Ecotoxicity Reference Value) of 31 mg/L, their 168-hr T/D concentrations would classify Na₂WO₄, 2H₂O, APT, AMT, WO₄ and WO₂⁻ as GHS Acute 3, but would not classify them under the EU CLP scheme. W metal and tungsten carbide would not classify under either scheme. Compared to NaSbO₃, Sn oxide and SnO₂ dissolved entirely as Sn(V) and Sn(III), which are their respective valences in these compounds. With Sb metal, Sb dissolution was primarily as Sb(III). For Sb₂S₃, the speciation data suggested a significant degree of Sb(III) oxidation to Sb(V) over 28 days. For NaSbO₃, Sb dissolved as Sb(V), since antimony is pentavalent in this compound. For Sn/C.SnO₂, the Sn/C.SnO₂ ligand appeared to stabilize Sn(III) in solution, with only a moderate amount of oxidation. Similar comments apply to the CH₂COO⁻ ligand in Sn(CH₂COO)₂, particularly at pH 6. On the other hand, Sn(III) released from SbCl₃, was readily oxidized to Sn(V). With pentavalent Sn in SnO₂, the speciation data indicated an initial small amount of Sn(III) that oxidized to Sn(V) over the 28 days. A comparison of the T/D data with the 6.9 mg/L acute ERV for dissolved Sn revealed that none of Sn metal and its compounds would classify under the EU CLP.

RA05-2
Transformation/dissolution of copper alloys: comparison of two anti-abrasion devices for massive sample testing
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In view of determining the environmental classification of copper alloys, the potential for metal releases from a range of copper alloys was assessed using the OECD Transformation/Dissolution (TD) test (2001). Metal releases from metals in massive and powder forms are a function of the surface area exposed to the media. Consequently, to assess comparative metal releases from copper alloys, there is a need to standardize the surface area exposed and to preserve the integrity of the alloy samples. The aim of this study was to define a protocol suitable to TD testing of massive forms of copper alloys.

Accordingly, two anti-abrasion devices were designed to protect the integrity of the alloy samples. The first device involves two polypropylene (pp) wheels attached to the ends of a warp wire sample, to avoid metal contact with the vessel walls. The second device is an epoxy jacket mounted around the sample; in this case the alloy surface exposed to the media was polished to assure a known and homogeneous surface quality and avoid effects of corrosion and passivation, proper of sample aging under uncontrolled environmental conditions.

The non-abrasion devices were applied to nine different copper/zinc and copper/nickel alloys and the samples were subjected to 7 days TD at pH 6. The T/D results of samples embedded in epoxy resin showed lower experimental noise compared to those for the polypropylene wheels and is therefore considered as a more appropriate methodology for transformation/dissolution testing of massive forms.

Microscopy studies of samples surface concluded that defects in the alloy surface during the wire production were responsible for the higher variability in the T/D results of the polypropylene wheels protocol, compared to the epoxy polished sample protocol.

The surface-specific metal releases from the alloy samples, using both anti-abrasion protocols, usually increase linearly with time, with faster dissolution rates for lead and zinc and lower rates for copper and nickel. The dissolution kinetics of lead in three samples, demonstrate a decrease in the metal release ratio as the tests progress, suggesting a decrease of lead from the alloy surface. For copper, the main component of the alloys, the dissolved copper concentrations measured in the alloy were between 0.04 and 2.05 µg/mm², compared with the values observed from pure copper samples (0.14 to 0.41 µg/mm²).

RA05-3
Transformation/dissolution of copper concentrates: effect of mineral composition on metal solubility
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In view of determining the environmental classification of copper concentrates, being complex, heterogeneous and variable inorganic substances, this study aims at understanding the relation between the elemental/mineralogical composition of some selected copper concentrates and the Transformation/Dissolution behaviour of these concentrates. The mineralogy of the samples, determined by X-ray diffraction and microscopy studies, revealed the presence various copper minerals: Bornite, Chalcocite, Chalcopyrite, Covellite, Digenite, Enargite and Tennenite.

The release rates and their associated factor concentrations contained from different copper ore body were ascertained and demonstrated the presence of Cu, Fe, Zn, Pb, Cd, Co, As, zinc and lower rates for copper and nickel. The dissolution kinetics of lead in three samples, demonstrate a decrease in the metal release ratio as the tests progress, suggesting a decrease of lead from the alloy surface. For copper, the main component of the alloys, the dissolved copper concentrations measured in the alloy were between 0.04 and 2.05 µg/mm², compared with the values observed from pure copper samples (0.14 to 0.41 µg/mm²).

RA05-4
Metal classification using a unit world model: assessing removal rates from the water column and remobilization from sediment with TICKET-UWM
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European Union (EU) regulations pertaining to Classification, Labelling, and Packaging (CLP) of chemical substances follow the United Nations Globally Harmonized System (UN GHS). Under this system, speciation, partitioning, and precipitation are recognized as critical elements in metal hazard classification. Guidance on environmental transformation/dissolution behaviour included in the EU CLP guidance document includes a provision for demonstrating removal from the water column to assess the “persistence” or lack of degradation of metals. In analogy to organic chemicals, “rapid degradation” for metals requires greater than 70% removal within 28 days. However, unlike organic chemicals, where removal from the water column occurs via degradation, metal removal occurs through changes in speciation (partitioning and precipitation) followed by sedimentation which transfers metal to the sediment. Therefore, in line with the GHS guidance, “rapid degradation” for metals requires one to demonstrate not only rapid loss from the water column, but also limited remobilisation potential from sediment.
A unit world model for metals in lakes, TICKET-UWM, has been developed that considers key processes affecting metal transport, fate, and toxicity including complexation by aqueous inorganic and organic ligands (e.g., DOC), adsorption to particulate organic carbon (POC), binding to biological receptors (biotic ligands), and transport of dissolved metals and solids between the water column and sediment. The TICKET-UWM was used to assess the rate at which metals (Cu, Pb, Zn, Ni, Co, and Cd) are remobilized from the water column in a generalized lake system through partitioning and settling. The model was also used to assess metal speciation changes in the sediment and the potential for metal remobilization from sediment.

Model results indicate that, in most cases tested, greater than 70% of the metal added to the water column was removed within 28 days. Results also suggest the potential for remobilization of metals is limited, particularly when acid volatile sulfide (AVS) is present to precipitate metals as metal sulfides.

RA06-5
A BLM probabilistic approach to integrate variability in the derivation of Water Quality Criteria at regional and local scales
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The biotic ligand model (BLM) is one of the more promising models allowing to derive Water Quality Criteria (WQC) based on true bioavailable fractions of metals. However, several physico-chemical parameters must be assigned for running BLMs (i.e. pH, major cations, DOC) and the operational use of BLMs can suffer several flaws because of:
- the lack of comprehensive data. National monitoring programs of water bodies were indeed not originally designed for BLMs application and, as a consequence, some datasets can be incomplete;
- the lack of variability. Rivers and lakes can indeed show great spatial and temporal variations. So far however, only single values were generally considered for describing variability of concern, and the high natural variability with time and along a river watershed was ignored.
The main objective of this study was then to investigate the potential of probabilistic approaches able to capture the uncertainty of variables of concern and the incompleteness of datasets for BLMs application on large scales. The methodology was tested on the Loire river watershed for copper, where different spatial scenarios were considered. Data availability for copper showed that a significant fraction of dissolved concentrations (about 50%) were below the limit of detection. In order to impute realistic values to these non-detects, ‘distributional’ methods were used. In addition, probabilistic risk assessment was also conducted at local scale (i.e. considering data collected at a given monitoring station only). In such a case, the number of available data can be reduced dramatically and frequentist statistics can be more subject to criticism. To overcome the problem of data scarcity, a Bayesian approach was proposed.

Results showed that PNEC values calculated with or without probabilistic approaches significantly differ, e.g. if non-detects are ignored, the risk index is above one (situation at risk), while it is below one if a distributional approach is considered (situation at risk). Similarly, in case of scarcity of data at local scale (i.e. at a given monitoring station), frequentist and Bayesian approaches led to results significantly different.

RA06-6
Accounting for both local aquatic community composition and bioavailability in setting local quality standards for metals
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Recent years have seen considerable developments in the ability to make water quality standards for trace metals more ecologically relevant by taking account of the effect of local water chemistry conditions on bioavailability. This prevents situations where a different level of risk is considered to acceptable at different sites due to changes in bioavailability which are not accounted for in the standard. We describe preliminary efforts to address an additional issue in the development of water quality standards which are specific to particular locations, by taking account of the composition of the local ecological community (the ultimate protection objective). This has been addressed through the use of field measurements to derive species sensitivity distributions (SSD) in sediments. An alternative approach, which combines a quality assessed community dataset with field measurements of the abundance of benthic macroinvertebrates to derive an SSD on the community which is either expected to be present, in the absence of anthropogenic pressures, or the community which is present at the sites. Specific standards are derived for zinc in an area impacted by historic mining activities. Site-specific targets for zinc, based on the macroinvertebrate ecology predicted or observed at a site, can be derived and can result in improved compliance compared to traditional monitoring methods and bioavailability-based EQS. In addition to zinc, the approach is likely to be applicable to other metals and possibly other types of chemical stressors (e.g. pesticides). However, the methodology for deriving site-specific targets requires additional development and validation before they can be robustly applied during surface water classification.

RA06 - Contaminated sediments in a changing environment
RA06-1
Bioavailability and beneficial use as primary demands for a management guidance of contaminated dredged sediments
E. Caste, B. Weiler, A. Scheffler
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Management of contaminated sediments is a key issue in order to establish a sound development of the Baltic Sea and contributing to the EU Strategy for the Baltic Sea Region (EUSBSR). This issue is of utmost importance according to Helcom and addressed by the BSR funded project SMOCs (Sustainable Management of Contaminated Sediments). The main delivery of SMOCs comprises a guideline, including tools for assessment of sustainability, and decision support. The purpose of this lecture is to present the draft guideline on sustainable management of contaminated sediments for dredging projects all around the Baltic Sea. This proposal is a result of the joint EU-project SMOCs under consideration of actual national and international regulations, integrating other projects as well as interests of stakeholders. For example, the participants of a workshop preferred a guidance document giving new ideas and an overview of options for dredged material management. Exact definition of the term of “dredged material” (when to call dredged material “clean”, “contaminated” or “hazardous”) and action levels were required. Emphasis was given to fulfill political demands as to avoid waste production. Therefore it was primarily recommended to assess the feasibility of beneficial use of the sediments. Bioavailability concept for the derivation of sediment quality standards has a challenge to foster this approach, because not the total amount of contaminants is of importance rather than the biological available part. Such risk assessment based on laboratory or in situ studies meets the request of the European Water Framework Directive to develop a toxicity-based bioavailability model to estimate the risk of sediment-associated contaminants. The purpose of an LCIA probably in combination with a Risk Assessment is to ensure that dredging activities are performed in an environmentally acceptable manner, use sound engineering techniques, which they are economically warranted and take sufficient consideration of long term effects. The choice of appropriate indicators is given in detail as part of a Decision Support Tool.

RA06-2
Natural attenuation in sediments
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Due to polluted groundwater in urban areas, sediments in urban water streams become polluted as well. This can cause pollution of surface waters. Natural attenuation of chlorinated hydrocarbons in sediment can be used to sustainably manage or remediate groundwater pollution. Due to the change in remediation procedures in the Netherlands from site specific remediation to area specific remediation, an approach based on natural attenuation will be increasingly considered. Provided that the risks of this approach can be controlled, natural attenuation processes in sediment can be a valuable contribution to area specific management and remediation plans. However, there are still some knowledge gaps about these natural processes. Also research methods to quantify these processes are lacking. And the possible ecological effects in sediment or surface waters are still unknown.
From the knowledge gaps, research questions have been defined. How are the most important processes related and can these processes be modeled? Where does biodegradation occur? How fast is this process? Can it be stimulated? Which techniques can be used for monitoring? Six polluted sites in three cities in the Netherlands were sampled, including 1 reference sample per site. Samples were either frozen in liquid nitrogen or the individual sediment layers were sliced and sampled in the field. Chemical and molecular (Q PCR) analyses have been performed in order to characterize the sludge and sediment.
The research has shown that in the toplayer of the sediment, which contains the highest organic matter content, anaerobic conditions are present. In this layer the microbial activity is higher than in deeper sediment layers. The dechlorinating capacity in this layer is higher than in deeper layers. However, in the toplayer, not only anaerobic organisms are present, but also aerobic and micro-aerophilics. This implies that microaerophilic conditions are present and chlorinated ethenes can be both aerobically and micro-aerobically degraded. In the lower, this has implications for the management of dredging material in this specific canal. Dredging of the canal would, at least temporary, decrease the dechlorinating capacity. This could cause an increase in chlorinated ethenes in surface water and result in ecological risks during a certain period of time. The rest of the results will become available in December and January.
Upper percentages were found for sediments than for soils, indicating that PCDD/F and DL-PCB are more important for the floodplain contamination.

Influence of the Elbe contamination through its tributaries could not be found. A comparison of Bio-TEQs with their respective Chem-TEQs for the sum of polychlorinated dibenzo- and biphenyls (PCDD/F) and dioxin-like polychlorinated biphenyls (PCBs) was performed. The Chem-TEQs accounted for 0.1 % and 11.9 % for the floodplain contamination. A multi-layer fractionation of three selected transect samples, which eliminated the moderately persistent pollutants, gave clear evidence that the majority of dioxin-like activity might indicate the influence of the tributaries on the contamination of the Elbe.

All freeze-dried samples were extracted by means of pressurized liquid extraction. Dioxin-like activities were determined via the EROD assay with RTL-W1 cells and in parallel via the H4IE-luc assay with the eponymous transfected rat hepatoma cell line. All samples showed elevated dioxin-like effects, except two North Sea samples, showing no effects in the H4IE-luc assay. Nevertheless, both bioassays gave a good correlation with Bio-TEQs between 1307 and 10462 pg g bw -1 . They identified the industrial city Lysa na Labem as the highest contaminated site and revealed the floodplain soils to be equally contaminated like the Elbe sediments. But a flood influence could only be supposed due to the missing flood data and a soil sampling depths that gave no information about freshly deposited matter during the flood 2002. An influence of the Elbe contamination through its tributaries could not be found. A comparison of Bio-TEQs with their respective Chem-TEQs for the sum of polychlorinated dibenzo- and biphenyls (PCDD/F) and dioxin-like polychlorinated biphenyls (PCBs) was performed. The Chem-TEQs accounted for 0.1 % and 11.9 % for the floodplain contamination.

A multilayer fractionation of three selected transect samples, which eliminated the moderately persistent pollutants, gave clear evidence that the majority of dioxin-like activity in these samples was caused by non priority and non-persistent pollutants.

Can flood events affect rainbow trout? The biomarker-cascade after exposure to PAHs in sediment suspensions

The major findings of our study were that CNT inhibited growth of green algae, but not due to direct effects, like reduced photosynthetic activity of the green algae, but mainly due to indirect effects, namely shading of light in turbid test suspensions and agglomeration of the CNT with algal cells. After the scientific facts presented in ES&T, the results of our study on effects of carbon nanotubes (CNT) on green algae were published in 2011 in the peer reviewed journal Synthesis and Environmental Science & Technology [1]. The press discussed the results very diversely: Taking over our message to interpretations far away from the scientific context.
Nonetheless, it is difficult to think that there may be a direct contact between those who do research and who makes the decisions: firstly, because in most cases there are citizens.

These works were conducted in the framework of a research project « How to use REACH. How the stakeholders approach REACH through technical classes'. Discussion of those intermediaries who have relationships with key stakeholders and are able to translate information for them so that they become understandable and translatable into action.

The German Federal Environment Agency runs a site for aquatic simulation in the very south of Berlin, which also includes a set of outdoor and indoor artificial pond and stream mesocosms (FS). A Network of Excellence (NoE) was recently formed in radioecology, a science concerned with the transport and effects of environmental radiation. The NoE was formed to combat several problems in radiocology that are not uncommon in many other disciplines: 1) a steadily decreasing funding base; 2) fragmentation of resources and infrastructures; 3) poor recruitment of young scientists; and 4) retirement of key personnel. Nine organizations from eight countries formed the NoE with goals of developing a sustainable, long-term integration of radiocology in Europe. The integration that was required by the scientists resembled, in the business world, a partial merger of divisions from within different organizations. We thus sought a business school that specialized in change management to help us with the integration. Our NoE became a special project for five of MBA students. This presentation highlights some of their findings. Foremost, the MBA team determined that to create a sustainable NoE, there had to be integration among the people. This included working towards a shared vision, understanding the cultural differences involved in the project, and sharing the same expectations about what the scientists and their respective organizations receive from the NoE. Studies from past attempts at mergers and acquisitions in the business world indicate that failure to integrate usually occurs because the fundamentals of change management are overlooked and/or taken for granted.

Our preliminary findings suggest that there needs to be a balance of "emotions" and "science" in communicating risks - the discourse of risk is tightly related to emotional reactions. Moreover, studies into risk perception found that emotional reactions often play a more significant role in perceiving risks than our cognitive judgement. While it is important to keep the process of risk assessment objective and science-based, the general public can be better informed from communicating risks with the costs and benefits clearly outlined.

Research findings and decision making: the case of renewable energy

Research findings and decision making: the case of renewable energy

V. Cellarari, A. Pizzallunga, S. Sala

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Scientific research can have a role in the promotion of more sustainable patterns of consumption and production because it can provide information aimed to raise awareness about the impacts of different behaviours and to support more sustainable choices from different kind of actors. The challenge posed to science in this context is to provide information that is effectively supporting decision making processes at different scales and that can be easily understood by all the stakeholders involved in the process (policy makers, entrepreneurs and citizens). In recent years the attention of citizens on the issues of sustainability, environmental impacts and sustainable behaviour has grown considerably. In parallel the demand for scientifically sound and transparent information upon which to base consumption choices and behaviours is growing among citizens.

Nonetheless, it is difficult to think that there may be a direct contact between those who do research and who makes the decisions: firstly, because in most cases there are no opportunities for direct contact (e.g. to citizens) and, secondly, because is necessary to translate the information resulting from scientific research in a language that is understandable. The lack of communication between science, policy and citizens communication can lead to not evidence-based decision making, lack of trust and unsustainable behaviour due to low level of information and awareness.

One possible way of success in environmental communication could be represented by the presence of those intermediaries who have relationships with key stakeholders and are able to translate information for them so that they become understandable and translatable into action.

We present a discussion about wood use as a renewable energy source: communication of the main scientific findings about its sustainability and environmental impacts associated to it in support to decision making in energy planning and energy use.

Challenges of integrating science and people within a network of excellence

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2IAE School of Change Management, Aix en provence, France

A Network of Excellence (NoE) was recently formed in radiocology, a science concerned with the transport and effects of environmental radiation. The NoE was formed to combat several problems in radiocology that are not uncommon in many other disciplines: 1) a steadily decreasing funding base; 2) fragmentation of resources and infrastructures; 3) poor recruitment of young scientists; and 4) retirement of key personnel. Nine organizations from eight countries formed the NoE with goals of developing a sustainable, long-term integration of radiocology in Europe. The integration that was required by the scientists resembled, in the business world, a partial merger of divisions from within different organizations. We thus sought a business school that specialized in change management to help us with the integration. Our NoE became a special project for five of MBA students. This presentation highlights some of their findings. Foremost, the MBA team determined that to create a sustainable NoE, there had to be integration among the people. This included working towards a shared vision, understanding the cultural differences involved in the project, and sharing the same expectations about what the scientists and their respective organizations receive from the NoE. Studies from past attempts at mergers and acquisitions in the business world indicate that failure to integrate usually occurs because the fundamentals of change management are overlooked and/or taken for granted.

[NOTE to organizers: This platform session is intended for a special session organized by F Brechignac and I. Linkov, (francois.brechignac@irsn.fr). I do not see it listed among the ‘topics’. Although the subject of this presentation seems to fit perfectly with SETAC’s conference theme of Integrating Science and People, I do not see where it might best fit among your topics. Below, I have listed F24....but welcome your suggestions as to other options. Thank you.]

Keep your boots muddy

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The German Federal Environment Agency runs a site for aquatic simulation in the very south of Berlin, which also includes a set of outdoor and indoor artificial pond and stream mesocosms (FSA) for eco-toxicological research (http://www.umweltbundesamt.de/wasser-und-gewaesserschutz/fsa/). Up to the present, 30 studies were carried out in that facility during the last 10 years. The results have been popularised via the official homepage, guided tours, conference posters, talks and sessions, scientific journals, magazines, newspapers, and TV features. In search for further means to reach a wider audience apart from ecotoxocological professionals and people interested in natural sciences, the idea of the artist Anne Rinn (www.anne-rinn.de) to stage an exhibition and to create a film entitled 'Keep Your Boots Muddy' was supported by the FSA team. Both exhibition and film pivot on the triangle nature-simulation-art with simulation trying to create artificial nature. The presentation will be the 10 minutes version of the German film with English subtitles.

RA09 - Focal species of birds and mammals and their ecological behaviour for refined risk assessments of plant protection products in Europe

RA09-1

Benefits of EFSA Risk Assessment for birds and mammals’ guidance document for ecological refinements

To harmonize a refined zonal risk assessment, the Northern zone has agreed upon the following:

1. Selection methodology is discussed using cereals and pome fruit orchards in Europe as case studies.
   - Diet guilds, feeding strata, body weight and food intake rate to ensure that a given focal species are representative to provide a robust risk assessment. The focal species include a wide range of bird species in different crops at relevant growth stages relevant for the use of the chemical applied. Focal species have been studied in 16 EFSA crop categories, mostly by the Plant Protection Product producing companies who register their products within Europe (BASF, BCS, Cheminova, DOW, GOWAN, Makhteshim, Irvita, Isagro, Monsanto).
   - The studies have been conducted in eight different countries spread across member states in the central and southern registration zones of Europe. The total number of survey sites and which the surveys of each study took place ranges from a minimum of two weeks to up to four months. Here we will present data of two crops (cereals and pome fruit) for two different periods representing different BBCH growth stages.

2. Modelling (body burden or ecological models) are not considered appropriate for higher tier risk assessment until validated models and guidance are available.

3. Identification of bird focal species in France for refined risk assessments for plant protection products
   - V. Pouliès, C. Andrade
   - ANSES, Maisons alfort, France
   - National Museum of Natural History, Paris, France
   - The refined risk assessment for birds and mammals might be based on different parameters such as measured residues in food items, and on behaviour and diet of focal species.
   - The EFSA Opinion (2009) provides generic focal species for the major crops, but when further refinement is necessary, focal species defined in the opinion as "real species that actually occur in the crop when the pesticide is being used" should be identified. The National Museum of Natural History in France has got a huge data base containing registrations of bird presence on the territory, based on field observations made by a large network of naturalists. A methodology has been built to identify the focal species on several groups of crops by crossing the information issued from the Museum database, the reparation of crops in France, protected studies provided by industry, and a literature review. The outcome of this work, presented as a compiled document, contains identified focal species per groups of major crops, their behaviour and feeding habits.

4. Bird focal species in crops according the EFSA - how to find the right candidates
   - J. Ludwigs, C. Wolf, C. Dietzen, P. Edwards
   - RIFCON GmbH, Hirschberg, Germany
   - tier3 solutions GmbH, Leichlingen, Germany
   - Syngenta, Bracknell, Berkshire, UK
   - According to EU Council Directive 91/414/EEC and Regulation 1107/2009, the effects of crop protection products on wild mammals and birds have to be assessed. For this reason crop-specific focal species candidates can be defined for different periods representing different BBCH growth stages. The total data base consists of 72 field studies of plant protection product producing companies who register their products within Europe (BASE, BCS, Cheminova, DOW, GOWAN, Makhteshim, Ivita, Isagro, Monsanto, Sharda and Syngenta). The studies have been conducted in eight different countries spread across member states in the central and southern registration zones of Europe. The total number of survey sites and which the surveys of each study took place ranges from a minimum of two weeks to up to four months. Here we will present data of two crops (cereals and pome fruit), and the most important value calculated on the basis of the raw data is the frequency of occurrence per field (FOField), which denotes the number of fields where a species was recorded as percentage of the total number of fields regardless of the number of individuals observed. Furthermore it is necessary to consider parameters such as diet guild, feeding strata, body weight and food intake rate to ensure that a given focal species are representative to provide a robust risk assessment. The focal species selection methodology is discussed using cereals and pome fruit orchards in Europe as case studies.

5. European distributions of farmland birds used as focal species for pesticide risk assessment
   - P.J. Edwards, C. Wolf
   - 'Rifcon' GmbH, Hirschberg, Germany
   - 'Tier3' solutions GmbH, Leichlingen, Germany
   - Risk Assessment guidance for birds and mammals in Europe has been described by EFSA [1]. The process is tiered. To refine risk assessment it is necessary to define focal species in different crops at relevant growth stages appropriate for the use of the chemical applied. Focal species have been studied in 16 EFSA crop categories, mostly by industry, in several EU member states. Here we present data for major crops the focal species have been determined in several MSs and this provides evidence of their distributions. Studies have not been measured in all crops in all Member States (MS) since there is room for extrapolation between zones and crops. The EU has established voluntary zonal work sharing for the registration and reregistration of plant protection products which have been described by SANCO/8896/2009 [2] starting it is reasonable to place MS in geographical zones (Zonal Approach) where there is greatest similarity in climate, crops and general conditions that may influence exposure to pesticides and hence the risk. The purpose of the presentation is to demonstrate how an evaluation of the distribution of focal species from these data can be done and to compare the distribution of focal species from these studies with the distributions for the same species provided by the European Birds Atlas database. To illustrate this approach, one crop example (cereals) will be used. The approach developed may allow extrapolation in line with the Zonal Approach, such that MS risk managers can have confidence in using refined exposure data for a single set of focal species applied to a crop within a zone or even across zones.
Small mammal communities in agricultural landscape in central Europe: review of long-term field data
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Little is known about general small mammal communities in agricultural landscape in central Europe. Most published data represent only a few months’ data in a specific habitat type focussing on a small region. This presentation will review data from several studies performed in the last decades in agricultural landscape across different regions in Germany and the Czech Republic. Data on the distribution of small mammal species in agricultural landscape including cropped fields, meadows and adjacent field structures like hedgerows and woodland are presented. The results of three data sets in comparison will focus on general conclusions and may help to interpret the spatial and temporal composition and distribution of small mammal communities in agricultural landscape in central Europe.

RA10-1 Global Mercury: Bridging science and policy

Mercury emissions in large Hg-polluted floodplain areas in Germany are under an underestimated problem: challenges for reliable risk assessments and implications for authorities J.R. Renkle
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Environmental pollution by mercury is a world-wide problem. Particularly floodplain ecosystems are frequently affected. One example is the Elbe River in Germany and its catchment areas; large amounts of Hg from a range of anthropogenic and geogenic sources have been accumulated in the soils of these flood plains. They serve as sink for Hg originating from the surface water of adjacent river. Today, the vastly elevated Hg contents of the floodplain soils at the Elbe River often exceed even the action values of the German Soil Conservation Law. This is especially important as Hg polluted areas at the Elbe River achieve several hundred square kilometres. Thus, authorities are coerced by law to conduct an appropriate risk assessment and to implement practical actions to eliminate or reduce environmental problems. A reliable risk assessment particularly with view to organisms (green fodder and hay production, grazing and wild animals) to avoid the transfer of Hg into the human food chain, requires an authentic determination of Hg fluxes and their dynamics since gaseous emissions from soil to atmosphere are an important pathway of Hg. However, reliable estimates of Hg fluxes from the highly polluted floodplain soils at the Elbe River and its tributaries, and its influencing factors are scarce. For this purpose, we have developed a new method to determine mercury emissions from soils at various sites. Our objectives were i) to quantify seasonal variations of total gaseous mercury (TGM) fluxes for floodplain soils at the Elbe River, ii) to provide insights into physico-chemical processes regulating these TGM fluxes, and iii) to quantify the impacts of the controlling factors soil temperature and soil water content on Hg volatilization from a typical contaminated floodplain soil within soil microcosm experiments under various controlled temperature and moisture conditions. Our study provides insight into TGM emissions from highly Hg-polluted floodplain soils in Germany and that those emissions are an underestimated problem. Current needs for reliable risk assessments, the induced implications for authorities, and future challenges will be discussed. The presented data will contribute to a better understanding of seasonal dynamics of Hg fluxes and its controlling factors. This presentation should be of large interest for a wide international audience, such as environmental scientists and managers, applied ecologists, and authorities.

Mercury in the Mediterranean: status and mass balance
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An interesting feature of mercury biogeochemistry in the Mediterranean is that several fish species from the Mediterranean show higher concentrations of Hg than same fish species in the Atlantic ocean, although the concentrations of total mercury in the open waters of both oceans are similar. Elevated Hg levels have been noted in environmental matrices from the Mediterranean region, adjacent to known mercury pollution, yet, the data do not clearly indicate that the effects of these anomalies have been transmitted to open waters or to lower trophic level species living in these waters. Recent studies indicated that the main source of MeHg in organisms in the coastal areas is related to methylation in sediments, while net mercury methylation in the open ocean occurs in the water column and is linked to organic matter regeneration promoted by the presence of sufficient light. Relatively large portion of mercury in waters is present as dissolved gaseous mercury (DGM), originating from photochemical, biologically mediated mechanisms and/or diffusion from deeper layer either due to biological and/or to tectonic activity which is typical of the Mediterranean region.

Recent studies on distribution and cycling of mercury in a mass balance were implemented. It has been shown that exchange with the atmosphere is the most important source of mercury for the water compartment. Measurements have shown that the evasion of Hg varied between the different seasons with the highest evasion during the autumn and an estimate of yearly evasion from the Mediterranean Sea surface was estimated to range between 250-350 Kmol/yr. Two important zones of MeHg productivity are reported in the Mediterranean Sea: one at the bottom of the euphotic layer and the other at the oxygen minimum in the thermocline. The proposed methylation and demethylation rates vary between 0.3-6.3 % day-1 and 6.5 -25 % day-1, respectively. Based on these values the estimated production in the euphotic zone is between 500 and 1000 Kmol/yr, and degradation was estimated to 720-1000 Kmol/yr. It has been shown that the total mercury exchanges at the straits are not unbalanced, while mercury methylation and demethylation rates vary between 0.3-6.3 % day-1 and 6.5 -25 % day-1, respectively. It has been also shown that Hg emissions to the atmosphere are not directly linked to the Hg emissions from industrial activities, but that both elemental and methyl mercury emissions are a result of natural biological activity.

Mercury and methyl mercury in the trophic chain of the Lagoon of Venice, Italy
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The Lagoon of Venice is one of the most polluted areas in Europe, due to the presence of the numerous coastal zones contaminated by mercury emitted from chemical industry (mainly alkali-chlor). Because of a long residence time of mercury, perpetually recycled between water and sediments, the transfer of mercury to biota in lagoons persists a long time after the reduction or elimination of Hg point sources. Previous studies in the Lagoon of Venice have demonstrated an elevated methylation potential, tide-driven MMHg transfer from sediments to water column and accumulation in some organisms. Here we report for the first time the initial results on Hg and MMHg bioaccumulation in the food web. Biota and sediment samples were collected in summer 2011 in the moderately polluted northern part of the Lagoon of Venice. Biota samples included pelagic and benthic
organisms from all trophic levels from primary producers to fish. Carbon and nitrogen isotopes were determined with a isotope ratio mass spectrometer (IRMS). Total Hg was analyzed using thermal combustion method (AMA 254) The Hg species were analyzed by species-specific isotope dilution and capillary gas chromatography hyphenated to inductively coupled plasma mass spectrometry (ICP-MS).

Based on δ²⁇N results the sampled organisms covered 3 trophic levels.

Total mercury concentrations in biota varied by nearly three orders of magnitude from 0.030 μg g⁻¹ d.w. (dry weight) in seagrass (Zostera marina) to 2.3 μg g⁻¹ d.w. in tissue of shrimp (Palaeomon elegans). There was a tendency of increasing Hg concentration with increasing trophic level, but the relation was not significant if all species were considered. MMHg concentrations varied between 3 (seagrass, phytoplankton) and about 2000 ng g⁻¹ d.w. (shrimps, fish) and the proportion of MMHg in total Hg was increasing with the trophic position of organisms. For the full set of data, the relation between MMHg and δ²⁇N values was best expressed by an exponential function (R²=0.59).

On average, the total accumulation of Hg and MMHg in the organisms in a moderately polluted area of the Lagoon of Venice increased by one order of magnitude for each of the three trophic levels. However, the deviations from this rule can be considerable for benthiic filter feeders (bivalve mollusks) and some fish apparently migrating from less contaminated areas. Results of this and follow up studies should provide a suitable model for risk assessment in more contaminated areas.

Dietary selenium at environmental concentrations reduces methyl mercury retention in some aquatic organisms at the lower trophic levels

Environmental relevant concentrations (<1 μg Se/g) of selenium in the food correlated negatively with half lives for methyl mercury. Selenium in the food also reduced the retention times for methyl mercury in the marine copepod Acartia tonsa, but in a less pronounced way than in the brown shrimp. In shore crabs Carcinus maenas no effect of selenium was found. The finding that there is a negative correlation between low, environmentally realistic selenium concentrations in the food and the half life for methyl mercury in brown shrimps indicates that selenium may play an active role for the biokinetics of methyl mercury in the environment. This is corroborated by similar findings in zebrafish Danio rerio [1] where small increases in the selenium concentration in the food also lead to a dose-dependent decrease in the retention of methyl mercury. The potential significance of the somewhat more limited effect of selenium at the lowest trophic levels (the copepods) and lack of effect in the shore crab needs more detailed elucidation.

Dietary selenium (as selenite, selenocystine and seleno-methionine but not selenate) reduced the retention on methyl mercury in the brown shrimp Crangon crangon.

Mercury pollution in China: releases, uses and impacts

China currently has the world’s largest intentional consumption as well as unintentional environmental release of mercury (Hg). Atmospheric emissions has been estimated to about 700 tons annually, accounting for one third of the global anthropogenic emissions. There are also large [but not quantified] releases to local soil and water environments. The intentional use of Hg in industrial processes and consumer products has been estimated at 1000 tons annually, roughly half of the global total. Mercury pollution is released to the environment by a wide range of sectors, including metallurgy, paper production, mining, power generation, non-ferrous metal production, and the cement and chemical industries. The industrial use of mercury in China has caused severe pollution incidents in the past. Today, as a result of past practices, high mercury levels are found in water, soil and rice near abandoned mercury mining and smelting areas.

The presentation gives an overview of the major issues regarding China’s Hg pollution issues, including releases, intentional use, environmental concentrations as well as human exposure.

RA11 - Guidance documents and guidelines for environmental risk assessment (ERA): needs, developments and progress

RA11-1

Ecological risk assessment of pesticides: linking non-target Arthropod testing with protection goals (ESCORT 3)

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The ESCORT 3 workshop (ESCORT: European Standard Characteristics Of beneficials Regulatory Testing) dealt with questions of the protection of “Non-Target Arthropods” in the context of the use of plant protection products in agriculture. It was the third ESCORT workshop that addressed this question. The Organising Committee put together a programme of discussion topics that were addressed at the workshop in plenary sessions alternating with work in sub-groups. This allowed for in-depth discussions on each of the four areas identified by the Organising Committee: a) Level of protection and testing scheme; b) Off-crop environment; c) Recovery; d) Field studies.

Approximately 60 participants registered for the workshop coming from authorities, the private sector, and academia. The participants of the workshop were assigned to one of the four sub-groups based on their knowledge and expertise, and regular plenary sessions gave participants the opportunity to comment on all areas under discussion. An opening plenary session provided background information with presentations from invited speakers. The ESCORT-3 meeting was held as a review and update of the previous meeting outputs based on current science. It also considered new issues and open points that had arisen in the interim period. The proceedings of this workshop will be finalized in the 2012 and this presentation aims at offering the audience an outline of these proceedings.

RA11-2

Development of OECD guidance on the conduct and evaluation of toxicity tests for endocrine disrupting chemicals

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The science of endocrine disrupting chemicals (EDCs) is developing, and two jurisdictions (European Union and United States of America) have now enacted regulations for the control of these substances. It was foreseen over a decade ago that such regulations would need to be underpinned by new toxicity assays relevant to human health and wildlife species, because the more traditional suite of internationally-standardised assays was insufficiently sensitive to known EDCs. In response to this perception, the Organisation for Economic Cooperation and Development (OECD) set up its Endocrine Disrupter Testing and Assessment (EDTA) programme to develop and validate new screens with some diagnostic capability for potential EDCs, as well as tests with apical endpoints sensitive to EDCs, several of which have now been published as OECD Testing Guidelines (TG). These include 2 in vitro procedures for detecting substances with potential to affect steroidogenesis (TG 456) or interact with the estrogen receptor (TG 455); 4 in vivo mammalian assays (TG 443, 441, 407 and 440) with diagnostic capability for, and/or sensitivity to, one or more of estrogens, androgens, thyroid disrupters and steroidogenesis disrupters (so-called EATS modalities); 4 in vivo fish assays (TG 229, 230 and 234; GD 148), also with EATS sensitivity; and one in vivo amphibian assay for thyroid-active substances (TG 231). In addition, OECD has developed, or is developing, a range of lifecycle or partial lifecycle assays with birds, fish,
amphibians and invertebrates which are able to measure the apical effects of EDCs without generally being able to diagnose causality. As well as briefly describing these assays, this paper will present a new OECD Guidance Document (GD) which helps users of the assays interpret their results, assists in reaching conclusions about whether test substances possess potential or actual endocrine disrupting properties, and provides advice about a possible further testing step should this be indicated. The basis of this GD is the need to evaluate all of the available information with the help of a weight-of-evidence approach, including existing data on similar chemicals, physico-chemical properties, results of in vitro tests, and in vivo toxicity in the same and other species. It will rarely be possible to conclude that a substance is an EDC solely on the basis of a single assay, so the GD will provide much-needed assistance to chemical companies and regulators alike.

RA11-3
ECETOC Ecotoxicological assessment of endocrine disrupting chemicals
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European regulations on plant protection produces, biocides and chemicals only support the marketing and use of chemical products on the basis that they do not induce endocrine disruption in humans or wildlife species. An ECETOC task force was formed to provide scientific criteria that may be used to identify and evaluate endocrine activity and disruption. This presentation focuses on wildlife species. For ecotoxicological assessments the key considerations include specificity, potency, population relevance and negligible exposure. Assessment of specificity is conducted within a study or species, to determine whether the endocrine mediated effect occurs at concentrations lower than those that cause other significant toxicity. Then the evaluation proceeds to consideration of specificity in relation to endpoints obtained in other taxonomic groups, which may drive the overall risk assessment. If the adverse effects are considered not specific the risk assessment is based on the non-endocrine endpoint. If specificity is confirmed, then the relative tolerance of the endocrine endpoint with an assessment factor based on potency. The endocrine-mediated NOEC/NOA/EL needs to be compared with other endpoints, e.g. by assessing the magnitude of the ACR, comparing the potency of the substance to a reference compound, duration of exposure that induces an adverse effect and the number of species in which the adverse effect is demonstrated. The protection goal of environmental risk assessments is the population and examples for relevant effects are: age at first reproduction, size of a reproductive event, frequency of reproductive events, duration of reproductive period, viability of young and sex ratio. Some effects are known to be responsive (and even sensitive) to, but not diagnostic of, endocrine modulation (e.g. fecundity, which can be affected by general toxicity). In such cases supporting information will be required to link the population relevant effect to an endocrine mechanism.

As there are currently no specified criteria for "negligible exposure" of wildlife species to plant protection products. Based on the wording in the regulation it is evident that negligible exposure must fall somewhere between "no exposure" (i.e. nominal concentrations of 0, or less than the limit of detection/limit of quantification) and a concentration representing an acceptable or low risk.

RA11-4
Environmental Quality Criteria (EQC): a comparison of methods under different regulatory regimes
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Environmental quality criteria (EQC) form the basis for legally binding environmental quality standards (EQS). The EQS’ are derived according to different European and national legal frameworks accompanied by technical guideline documents (TGD). Within European chemical and water regimes the TGDs are currently streamlined at European level. This harmonisation of methods is likely to influence both, the other sectors of environmental policy on the European level as well as the existing national risk assessment schemes.

The German Environment Agency has subjected the standards currently used under the German REACH Regulation to further scrutiny. In the context of the UNECE concept for terrestrial ecosystems, the comparison included the legal frameworks and procedural mechanisms for quality assurance. The methodology analysis comprised the normative framework, case studies and interviews with experts in the field. A key finding was the relevance of the GD, which had been developed to support risk assessment. The GD was based on the EU risk assessment concept and was considered a valuable tool.

RA11-5
Representativeness of Eisenia fetida for the environmental risk assessment of pesticides to soil organisms
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The sole routine testing of the standard earthworm Eisenia fetida for the terrestrial risk assessment of pesticides has been under much debate since other soil invertebrates may be more sensitive than this standard test species. Low availability of laboratory toxicity data for taxa other than E. fetida has greatly hampered previous sensitivity comparisons. In the present study, the relative tolerance of the endocrine approach was applied to enable comparing toxicity thresholds for main terrestrial taxonomic groups and pesticidal types of action (insecticides, fungicides, herbicides, and other) separately. Analyses confirmed previously reported lower and higher sensitivity of collembolans to fungicides and insecticides, respectively. However, various other discrepancies in susceptibility relative to Trel values. For example, arachnids and isopods were found to be more sensitive to insecticides, and nematodes to fungicides, as compared to E. fetida. Implications of study findings for the terrestrial risk assessment of pesticides are discussed.

RA12 - Health and environmental risk assessment of pesticides and biocidal products
RA12-1
Information requirements under the Biocidal Products Regulation and their implications for environmental risk assessment, authorities and applicants
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As of 2013, the current regulatory framework, the Biocidal Product Directive (BPD), is going to be replaced by the Biocidal Products Regulation (BPR). The upcoming regulation will encompass a wide range of regulatory changes. Union-wide authorisation of products, the obligation to substitute active substances with less-hazardous equivalent alternatives, as well as an exposure-based data waiving represent major changes that will affect both authorities and applicants. A further major change concerns the amount of quantitative and qualitative information to be submitted by applicants for both active substances approval and biocidal products authorisation. The BPR requires more compulsory information and exhibits a more extensive list of case-dependent additional information requirements when compared to the BPD. This could represent a major challenge for the applicant, but has to be weighed against the aim to improve hazard and risk assessments in a resource-efficient manner. Current (BPD) and future (BPR) information requirements are compared and discussed and the significance for environmental risk assessments is estimated. In addition, economic implications for applicants are discussed.

RA12-2
Proposal for a harmonized assessment of the mixture ecotoxicity of biocidal products
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A new physiology-based pharmacokinetic model for predicting mammalian tissue distribution of pesticides
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Physiology-based pharmacokinetic (PBPK) models are a type of mass-balance model used to predict the concentration profile of chemicals in the blood and tissues of a living animal. PBPK models are based on four main processes: absorption, distribution, metabolism, and excretion (ADME). Three of the ADME processes are strongly dependent on chemical partitioning properties; absorption, distribution, and excretion. A common approximation to describe the partitioning properties involved in these processes is to use a surrogate for storage lipids to estimate the lipophilicity and to assume that the sorption capacity of membrane lipids and proteins is related to the fraction of those phases that have a storage lipid-like sorption capacity. For highly lipophilic, non-polar chemicals the predictions are quite accurate. However, polar chemicals and chemicals with a weak bond with hydrogen and acceptors can deviate significantly. A more robust method with regard to neutral polar chemicals is a poly-parameter linear free energy relationships (PPLFER). In PPLFER equations explicit consideration is given to the different molecular level interactions that may exist between a solute and the solvent molecules of the phase in which it is sorbed, specifically dipole interactions, hydrogen bonding, and van der Waals forces.

An improved PBPK model for predicting total mammalian body burden and tissue distribution of neutral organic chemicals is developed. Partitioning to blood and tissues is built up from their basic as described by appropriate PPLFER equations. The model was calibrated and validated on biomonitoring, occupational exposure and epidemiological studies available in the literature. The model was subsequently applied to a dataset of pesticides with experimentally determined values for the solute and that the concept of Concentration addition is a suitable method for that. Therefore, using animal data for exposure characterization (mainly based on intended use in BPD product types) the second step covers potential effects. The scores from both steps are combined and used to prioritize compounds. In a first step it is evaluated in which environmental compartment a compound should be investigated (e.g. water, sediment, biota, soil). This evaluation is based on use patterns (product type specific emissions) and substance specific properties relevant for the compartment regarded (e.g. partition between compartments, persistence or BCF). The procedure was tested with a set of 80 biocides which are either already authorised biocides (BPA Annex I) or candidates (biocidal substances currently in the BPA review programme). The plausibility of the prioritisation is discussed with regard to the compiled monitoring data as well as to prioritisation results from other studies.
A new modeling approach was designed to account for pesticide residues in various food crops as source for human pesticide intake. Modeled residues are compared with measured concentrations of 12 different pesticide-crop combinations and correspond well with total crop-specific residual errors ranging between a factor of 1.5 for lettuce and a factor 19 for rice. Intake fractions calculated per unit mass of applied pesticide for 121 substances applied to all crops but potato are usually in the range of 10^{-2} and 10^{-8} kg intake per kg applied for typical times between application and harvest. Intake fractions obtained after direct application were 1 to 5 orders of magnitude higher than intake fractions estimated for indirect emissions, i.e. fractions lost to air and freshwater during application.

Main factors influencing the fate behavior of pesticides are the degradation half-life in plants and on plant surfaces, the residence time in soil as well as the time between pesticide application and harvest. A simplified model based on the most influential input variables enables the prediction of residues within a factor of 10 of those calculated with the complex model. Highest impacts are expected for herbicides and fruit trees with usually high intake fractions and consumptions, while roots and tubers only contribute little due to very low intake fractions. Substitution scenarios enable us to reduce health impacts by choosing alternative pesticides with similar ability to control unwanted pests, but with lower toxicity. However, substitution must be discussed separately within each pesticide target class.

RA14-1
Effects of scale on pesticide loss pattern and ecosystem services
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RA14-2
Exposure and ecological risk assessment of herbicides in Japan: validation and factor analysis for predicted concentrations of herbicides by the geo-referenced multimedia environmental model G-CIEMS
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Kitsatsuo University, Towada, Japan

Koriyama Women’s University, Koriyama, Japan

Prefectural University of Kumamoto, Kumamoto, Japan

The predicted environmental concentration (PEC) is calculated based on fate models or survey results. Pesticides are characterized using limited time points and places, hence for environmental风险 assessment is it important to predict temporal-spatial variations of the exposure concentrations. The multimedia environmental fate model G-CIEMS (Grid-Catchment Integrated Multimedia Modeling System) based on Japanese GIS data was developed in the past. In addition, emission estimation methods for herbicide use in paddy fields were developed that are applied to calculate temporal-spatial variations of herbicides concentrations in river waters for the total area of Japan. The model simulations were validated using field survey data from seven rivers. In this study, we focused on the analysis of factors which contribute to the accuracy of model predictions in order to improve the reproducibility of model results. The emission estimation method was divided into following three phases. In the first phase, used amounts of each herbicide formulation, which is the commercially available herbicide product, were predicted for each day for each prefecture. In the second phase, exposure of concentrations for one herbicide in paddy fields and the daily emission rate to air and water. In the third phase, we allocated emission amounts of herbicides to GIS segments based on land use data. Finally we calculated environmental concentration for all pesticides for the total area of Japan by the G-CIEMS model. We performed field survey from April 2009 to July 2009 for validation. The maximum concentrations were compared between prediction and observation for 166 pairs from total 173 pairs (= 7 river sites x 23 herbicides). For compound-or site-related average, more than 70% of the pairs had a prediction error of less than one order of magnitude. Based on comparison of the several phases, the predictions for higher accuracy herbicide group and lower accuracy one, degradation rate was significantly higher in the lower accuracy group with p < 0.05. We confirmed our model have high accuracy for predicting herbicide concentration variations in river for several sites and several herbicides. For improving our method, it is important to improve actual condition of degradation mechanisms of herbicides in the environment.

RA14-3
Linking exposure and effects of pesticides using passive samplers and the SPEARpesticides bioindicator - a case study in Central Germany, 2010
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Pesticides have always been an important stressor for non-target organisms, and today's modern pesticides are no exemption. Our investigations show the still high impacts from pesticides on freshwater communities in selected Central German agricultural landscapes, despite continuous attempts to reduce any unintended effects of the pesticides on the environment.

The study took place in the Bode river catchment located in the TERENO Harz/Central German Lowland Observatory, Central Germany, during the peak pesticide application period in 2010.

At 19 sampling sites along six streams, passive samplers of the type Chemcatcher® were deployed for 2 to 3 weeks to detect any pesticides originating from agricultural field run-off.

For each site, the composition of the aquatic macroinvertebrate community was established and the ratio of pesticide sensitive taxa was calculated according to the bioindicator system SPEARpesticides (SPEAR value; SPEAcies At Risk).

The deployed passive samplers detected 16 pesticides in very low concentrations ranging from 0.12 ng to 48.49 ng, proving themselves a reliable tool for the detection of chemicals in surface waters.

Toxic units (TU) were initially calculated for the obtained weight-based average pesticide concentrations (TWA) and later re-calculated for realistically estimated peak exposure time frames of 24 hours and 6 hours, respectively, based on the individual soil organic carbon-water partitioning coefficients (Koc) of all detected substances. The range of TU's shifted from previously 7.73 to 3.4 to now -6.7 to -2.0.

443 Macroinvertebrates belonging to 69 taxa were collected. A simplified model based on the most influential input variables enables the prediction of residues within a factor of 10 of those calculated with the complex model. Highest impacts are expected for herbicides and fruit trees with usually high intake fractions and consumptions, while roots and tubers only contribute little due to very low intake fractions. Substitution scenarios enable us to reduce health impacts by choosing alternative pesticides with similar ability to control unwanted pests, but with lower toxicity. However, substitution must be discussed separately within each pesticide target class.

RA14-4
Spatially-explicit exposure and ecological risk modeling tools: SEEM and FISHRAND
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We report on two wildlife exposure models that incorporate the impact of chemical distribution in the environment, habitat suitability relative to areas of contamination, and foraging behaviors of the modeled species. The Spatially Explicit Exposure Model (SEEM) is being developed for the US Army to improve the realism of terrestrial wildlife exposure modeling, SEEM tracks exposures for all individuals in a user-defined population rather than evaluating a single representative individual. Foraging for each individual is guided by habitat suitability preferences. As a result, individuals are less likely to forage in areas where the habitat suitability is low. Also, users may select two foraging strategies: a free-ranging strategy and a static home range strategy. The model generates population-effects curves. The aquatic model, FISHRAND (FR), is a mechanistic, time-varying bioaccumulation model. The second-order probabilistic model incorporates both sediment and water sources to predict the uptake of organic chemicals based on prey consumption and food web dynamics. The Monte Carlo probabilistic approach allows users to distinguish between sources of uncertainty and variability in predicted fish body burdens. The model allows for more realistic exposure estimates by incorporating data on fish home range, attraction factor (e.g., habitat suitability), and relative abundance. Users can specify preferred habitat areas relative to the contamination profile at the site. Both models offer assessors the tools necessary for advanced exploration of risk drivers and portions of a site in which habitat overlaps with chemical concentrations (and conversely areas where chemicals are present, but habitat is limited).

RA14-5
An agent-based woodpigeon population model used to estimate pesticide exposure in realistic landscapes
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Population modelling is a recommended method to refine risk assessment after the pesticide has failed the first-tier step. We constructed a spatially-explicit agent-based framework (SkyPig) with models of two species: skytler (Alauda arvensis) and woodpigeon (Columba palumbus) that can be used for population-level assessment of exposure
and effects of pesticides. In our model the birds are characterised by state variables changing dynamically as an effect of their interaction with other agents, environmental resources and time. The common algorithms (mortality check, managing the energy budget, foraging and conducting seasonal activities) operating on these variables result in representation of diverse patterns observed in real ecosystems: population dynamics over the years and foraging patterns including choice of feeding grounds and flocking. The TK/TD model explicitly reflects the patterns observed in data from density regulation studies. The distinctive property of our model is the landscape representation: natural structures (like fields or hedgerows) read from GIS maps are implemented as single landscape units without the need for an artificially created grid of hexagonal or square cells. In this study we present the exposure assessment for a realistic landscape scenario for two fictitious pesticides: pesticide A used as a cereal seed treatment and pesticide B used as a spray applied to oilseed rape. Woodpigeons are known to forage extensively on both cereal grain and oilseed rape leaves and therefore the use of these pesticides potentially exposes them to risk of poisoning. The model predictions on woodpigeon exposure in terms of toxicity-exposure ratios (TER) values obtained by individual birds are compared with TER values calculated for pesticides A and B as used in first-tier exposure model and refined exposure model used in higher tier risk assessment assuming PT and PD values for woodpigeons foraging on sown cereals and oilseed rape leaves.

RA1-4 Accumulation of trace metals in a complex world, validation of a spatially explicit model: BERISP

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In this study we present the exposure assessment for a realistic landscape scenario for two fictitious pesticides: pesticide A used as a cereal seed treatment and pesticide B used as a spray applied to oilseed rape. Woodpigeons are known to forage extensively on both cereal grain and oilseed rape leaves and therefore the use of these pesticides potentially exposes them to risk of poisoning. The model predictions on woodpigeon exposure in terms of toxicity-exposure ratios (TER) values obtained by individual birds are compared with TER values calculated for pesticides A and B as used in first-tier exposure model and refined exposure model used in higher tier risk assessment assuming PT and PD values for woodpigeons foraging on sown cereals and oilseed rape leaves.

RA1-15 Linking exposure to effects in environmental risk assessment

RA1-1 Development of a toxicokinetic/toxicodynamic model for the sublethal endpoint growth of a synchronized Scenedesmus vacuolatus cell population

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Most common ecotoxicological tests assess the toxic effects by exposing the organism with high dose and short exposure time under laboratory conditions. Process-based toxicokinetic/toxicodynamic (TK/TD) models may be used for extrapolation to chronic toxic effects under field conditions such as fluctuating and pulsed exposures. A TK/TD model simulates the temporal course of the endpoint concentration in the organism and the cause of the toxic effect. TK/TD models describe the sublethal endpoint growth of unicellular algae cell populations exposed to toxicants.

RA1-2 Toxilogical model of the sublethal endpoint growth of a synchronized Scenedesmus vacuolatus cell population

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In this study we present the exposure assessment for a realistic landscape scenario for two fictitious pesticides: pesticide A used as a cereal seed treatment and pesticide B used as a spray applied to oilseed rape. Woodpigeons are known to forage extensively on both cereal grain and oilseed rape leaves and therefore the use of these pesticides potentially exposes them to risk of poisoning. The model predictions on woodpigeon exposure in terms of toxicity-exposure ratios (TER) values obtained by individual birds are compared with TER values calculated for pesticides A and B as used in first-tier exposure model and refined exposure model used in higher tier risk assessment assuming PT and PD values for woodpigeons foraging on sown cereals and oilseed rape leaves.

RA1-5 Chronic effects on pairing behaviour and reproduction of Hyallela azteca following pulse exposure to permethrin

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Cascades, such as algae cell growth and algae cell reproduction, within a damage progress. Consequently, chronic toxic effects under field conditions may be simulated based on our mechanistic interpretation of algae life-cycle process and toxic effects on algae populations. Moreover, the TK/TD model has the potential to link several effect processes.

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Recently, research on accumulation of contaminants to higher organisms has focussed on several environmental factors that may affect food web accumulation. Abiotic factors, species specific traits and habitat have been described to affect accumulation patterns. This implies that spatial variation in environmental factors may play an important role in modulating accumulation. In the current presentation we will present a spatially explicit accumulation model (www.berisp.org), with specific focus on validation of results with field data. The model includes two types of food webs, an omnivorous and an herbivorous one. At the top of the omnivorous food web are two birds species as final receptors: the little owl (Athene noctua) and the blackbird (Turdus merula). Bovine grazer is the consumer in the herbivorous food web. For this study, three field cases were available to validate the models results. For small mammals, data from two case studies are available: the Metalurop Nord area, near a former Pb and Zn smelter in the North of France, and the Afferdensch and Deetsche Waarden (ADW), a metal-contaminated floodplain in the Netherlands. For the bovine grazers, results from a case study from Hageveen, Northern Netherlands are available. In that case, two herds of cows were followed in a natural area, and their feeding behaviour was monitored. Preliminary results on small mammals show that in the Metalurop Nord case the general pattern of the measured concentrations is reflected in the modelled concentrations: shrubs: bank vole – wood mouse > common vole. The differences between measured and modelled concentrations are higher for the bank vole. For the wood mouse and shrews, however, the modelled concentrations are higher. For the common vole, this is the other way around. Difference between modelled and measured concentrations are not significant for the bank vole. The model assumptions may be explained by differences in the assumed diet. In the ADW case, modelled concentrations in bank voles and wood mice are similar to the measured concentrations, as is also the case for the beetles. In the presentation, more detailed information on other receptors will be provided, including the effect of inclusion of spatially explicit foraying.
These differences resulted in substantial differences in population recovery times. Recovery after 16 day exposure to LC50 of diazinon took the longest, followed by recoveries for the other half, we used a logistic dose-response model. Simulated populations were exposed to 24h, 96h and 16 day LC50 of diazinon, chlorpyrifos, carbaryl and pentachlorophenol on May 1st in the simulated year. Population recovery was compared in populations where we accounted for TK-TD processes, hereafter termed TDM-populations, and those where we used a dose-response model for survival, termed DR-populations.

In conclusion, accounting for toxicokinetic-toxicodynamic processes results in differences, based on different pesticide characteristics, in magnitude of mortality and subsequent recovery times and yielded, on average, longer recovery periods.

Here we explore the joint impact of intrinsic sensitivity and pesticide specific factors on the population recovery. We developed an individual-based model (IBM) to simulate the population and the subsequent recovery of amphipod populations exposed to four pesticides in different exposure scenarios. Pesticide induced mortality was implemented with two different models. Toxicokinetic-toxicodynamic processes were accounted for by implementing the threshold damage model for survival in half of the treated populations. For the other half, we used a logistic dose-response model. Simulated populations were exposed to 24h, 96h and 16 day LC50 of diazinon, chlorpyrifos, carbaryl and pentachlorophenol on May 1st in the simulated year. Population recovery was compared in populations where we accounted for TK-TD processes, hereafter termed TDM-populations, and those where we used a dose-response model for survival, termed DR-populations.

Calculations of the mortality rate in populations exposed to chlorpyrifos, resulted in much more severe mortality in TDM-populations, when compared to DR-populations. These differences resulted in substantial differences in population recovery times. Recovery after 16 day exposure to LC50 of diazinon took the longest, followed by recoveries after chlorpyrifos, carbaryl and pentachlorophenol.

In conclusion, accounting for toxicokinetic-toxicodynamic processes results in differences, based on different pesticide characteristics, in magnitude of mortality and subsequent recovery times and yielded, on average, longer recovery periods.

Linking pesticide exposure to spatial dynamics: an individual-based model of wood mouse populations

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In pesticide risk assessment, risk is defined as a result of hazard and exposure. The less time animals spend in treated fields the less they will be exposed to pesticides and the risk is thus lower. Therefore, the spatial and temporal distribution and behaviour of non-target species are important in risk assessment. We studied the relationship between the spatial and temporal dynamics and the level of exposure by constructing a spatially explicit individual-based population model, using wood mice (Apodemus sylvaticus) on arable fields typical of the UK as an example. The model was constructed based on literature data on wood mouse life-history traits and behaviour. To capture the presence or absence of wood mice in certain fields on certain days, nesting and foraging behaviour and the corresponding movements were represented phenomenologically. Additionally, crop rotation and farming practices affecting the wood mice’s behaviour were included. The model is designed to link pesticide exposure and farming practices to the exposure movement and location of individual mice to study the effects of exposure at the population level. We briefly describe the model and then use two example scenarios to demonstrate the potential use of the model for ecological risk assessment of pesticides, addressing the question: how is the (i) spatial and (ii) temporal distribution of the mice, depending on crop type and season, related to pesticide exposure?

Monitoring data and post-registration studies: generation, compilation and use in the environmental risk assessment and management

Pre and post-authorisation monitoring for pesticides focussing on birds and mammals - recent developments from the SETAC environmental monitoring action group

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Bird and mammal risk assessments for individual populations carried out under EU Regulation 1107/2009 routinely use the relevant guidance document issued by EFSA (EFSA, 2009). This guidance outlines procedures of toxicity and exposure assessments for lower tiers. If concern is raised regarding lower tier assessments it may be possible to refine the risk assessment and although a range of options are available, detailed guidance is lacking as regards how to proceed. One possible refinement mentioned in EFSA (2009) is the use of field studies where ‘field studies’ refers both to studies of effects following experimental pesticide applications (i.e. applications made as part of a regulatory study) and also to ‘active monitoring’ of effects following applications of authorised products in agricultural practice. EFSA (2009) also highlights the potential usefulness of ‘passive’ wildlife incident monitoring or surveillance, involving investigation of suspected incidents reported by farmers and members of the public. The Environmental Monitoring Action Group for Pesticides (EMAG-PEST) of SETAC has been investigating the range of both pre and post-authorisation studies that have been conducted as well as the experience gained, with a view to consolidating ‘best practice’.

Post-authorisation monitoring for mammals, birds and insects - wildlife incident investigation scheme - England

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Food and Environment Research Agency, York, United Kingdom

The Wildlife Incident Investigation Scheme (WIIS) is a reactive surveillance scheme that monitors the suspected pesticide poisoning of wild animals, companion animals (pets) and beneficial insects. The suspected pesticides include plant protection products and biocides used to control vertebrate pests and similar schemes operate in Europe, Wales, Scotland and Northern Ireland. WIIS is partly funded by a levy on pesticide sales in the UK and it is co-ordinated by the Chemicals Regulation Directorate of the Health and Safety Executive (HSE), which is the lead authority on pesticide legislation. It has operated within a legal framework since the Control of Pesticides Regulations (COPR) 1986 and given this longevity and funding arrangements, it is probably unique in the world. The results from WIIS form part of the pesticide regulatory process and are reported quarterly on the internet. The majority of poisonings involve the intentional, illegal use of pesticides and where there is an infringement of legislation on pesticides or the environment, appropriate enforcement action may be taken by the Police, HSE or the local authority. How WIIS operates and the results of investigations into suspected poisonings in England will be discussed. This will focus on investigations where pesticides are used for an intended purpose. For example, honeybee poisonings from spray applications or feral bee treatments and slug pellet applications and rodent control for incidents with mammals and birds. The extent and possible reasons for the intentional, illegal use of pesticides will also be highlighted. Due to improved analytical methods that were introduced in 2010 (unpublished), WIIS has reported an increase in the number of bee incidents where multiple pesticides and/or very small pesticide residues have been confirmed. It is unlikely that these were the cause of death of the bees, but pesticides found include thiacloprid, deltamethrin, chlorpyrifos, fipronil and propiconazole. The agricultural use of pesticides may not be involved in some of these incidents and have wood treatments, amateur garden uses, or pet animal treatments are suspected. An effective, comprehensive and consistent approach to a monitoring scheme is an expensive commitment and a collaborative project among the major disease and contaminant monitoring schemes in the United Kingdom is now facilitated by the Wildlife Disease & Contaminant Monitoring and Surveillance WILDCOMS Network.
RA16-3
Bee health in Europe - facts & figures, A OPERA document
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2Ministry of Agriculture, Paris, France
3North American Pollinator Protection Campaign, San Francisco, United States of America
4National Bee Unit, York, United Kingdom
5Syngenta, Bracknell, United Kingdom
6Benaki Phytopathological Institute, Athens, Greece
7Bayer Crop Science, Monheim, Germany
8Dow AgroSciences, Latchmore, United Kingdom
9Apiculture Research Institute, Bucharest, Romania
10Julius Kühn-Institut, Braunschweig, Germany
11Declines of managed honey bee colonies and also of some wild bee species have been reported by many countries, leading to intensive work and actions in the areas of research and regulations. Declines in pollinating insect numbers can have significant adverse effects ecologically on the diversity of plant species and economically in the productivity of crops. However, up until now, the status and relative importance of the stress factors that may affect bee populations have been relatively unclear and, in many instances, widely disputed.
In this context, OPERA, has undertaken to produce an updated review on the issue of honey bees and pollinators in Europe, with some highlights to other continents, which would cover ecological and economical aspects related to these species in relation to agriculture. The expert invited have gathered the latest information available on the factors influencing the health of both managed honeybees and populations of native wild bees, including solitary and bumble bees. The main conclusions indicate that the honey bee can cohabitate with modern agricultural practices provided necessary precautions are taken to maintain viable food resources for bees and avoiding practices that may cause adverse effects. These precautions include the design of agricultural landscapes and the implementation of practices that account for the presence of pollinators. Essential developments also concern the availability of effective and regulated veterinary compounds to help beekeepers eradicate the most important pests from apiaries.
An analysis of beekeeping activity in its economical context is also provided. Finally, modern agriculture and beekeeping demands better technical knowledge and a critical lack of training and communication to better accompany the updates in science and technology to the farm and the field is identified.
The case of wild bees may be considered to be very similar to that of the domesticated honey bee albeit far less well documented. Recommendations are emitted towards all those involved in agriculture, bee keeping regulatory authorities and research, which should be communicated to all as the effectiveness of the actions will rely on their common effort to implement them.

RA16-4
Contamination of flowering crops by insecticidal dust drift - effects on honey bees (Apis mellifera L.)
JKL, Braunschweig, Germany
In 2008 a large-scale honey bee poisoning in parts of southern Germany occurred during sowing of maize. This incident was caused by contamination of flowering bee forage plants with dust from the insecticidal seed-dressing containing the active substance Clothianidin. Since early 2009, practical and large-scale drift experiments during sowing insecticide treated seeds were realized to investigate the link between abrasion potential of treated maize and oilseed rape seeds (determined by Heubach values), dust drift and resulting residues in adjacent flowering crops as well as the effects on honey bees. In ‘worst case’ scenario experiments bee colonies were set up in semi-field and field trials along the edges of the drilled area (treatment) to study the impacts of dust drift on mortality, foraging activity and brood development in bee colonies (exposure to dust during sowing and contaminated pollen and nectar) using drift-reduced pneumatic sowing techniques. Drilling was conducted during bee flight activity, so foragers were continuously exposed to dust. Two control variants were set up with hives in about 50 m (control) and more than 500 m (remote) distance to the exposed forage plants.
No adverse effect on bees and bee colonies were detected after raving sowing in 2009 and 2011. However, during maize sowing in 2010 and 2011 bee mortality was clearly increased.
Semi-field experiments with manual application of insecticide-loaded maize dust in Phacelia (Phacelia tanacetifolia Benth.) were carried out to analyse the impact of different rates of the active ingredient (0.5 g a.i./ha and 2.0 g a.i./ha Clothianidin) and different particle sizes (x ≤ 160 µm, 250 ≤ x ≤ 450 µm, x > 500 µm) of dust on mortality, foraging activity and brood development in bee colonies.
In contrast to the other dust fractions, at the same rate of Clothianidin for fine dust particles ‘x ≤ 160 µm’ significant mortality was detected. Studies on different rates showed effects on mortality only for the higher rate, whereas no differences were detected between the low rate and the untreated control.

RA16-5
Exposure of soil organisms to plant protection products - Monitoring the vertical niche differentiation of soil microarthropods in an arable field in the course of a year
Bayer CropScience, Monheim, Germany
Contamination of flowering crops by insecticidal dust drift - effects on honey bees (Apis mellifera L.)
JKL, Braunschweig, Germany
In this paper it is shown that the contamination of flowering crops by insecticidal dust drift during maize sowing in 2010 and 2011 bee mortality was clearly increased.

RA16-6
Use of groundwater monitoring data for existing agrochemicals to support re-registration
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In order to fulfill regulatory requirements for agrochemicals in the EU, the predicted environmental concentrations in groundwater (PEC Garner) are estimated using FOCUS models. Depending upon the uses to be registered, up to nine groundwater scenarios are modelled. The resulting concentrations are compared to a non-health-based cut-off criterion of 0.1 µg/litre. This modelling is designed to be conservative and thus tends to overestimate the concentrations in even the shallower aquifer. Recent revisions to the criteria governing the selection of modelling endpoints, such as the FOCUS Kinetics guidance, have tended to increase the conservative nature of the modelled PEC Garner. As increasing numbers of agrochemicals will not pass this arbitrary assessment step in the future, it is necessary to develop acceptable higher tier methodologies to refine the modelled output using real-life retrospective groundwater monitoring data. Data from a number of such studies with the maize herbicide, terbuthylazine, will be described and the potential acceptability of such data sets for the regulatory process will be discussed with special reference to key criteria that must be met for the data to be considered sufficiently robust to be used. Implications of the application of groundwater monitoring study data as a higher tier of assessment will be discussed.

RA17-1
A close look at the temperature-dependent chemical toxicity to aquatic organisms and its implication on derivation of water quality guidelines for protecting aquatic life
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The anticipated anthropogenically-driven climate change not only can increase the average air and water temperatures and prolong the hottest period, but also result in
increased incidents of temperature extremes that will have profound implications on the toxicity of chemical contaminants and hence their ecological risks to aquatic organisms. In this talk, I will comprehensively examine and discuss the mechanisms of temperature-dependent chemical toxicities to aquatic ecotoxothems based on both literature review and empirical laboratory studies. Examples will be drawn from an array of marine organisms including amphipod, copepod, diatom, and fish after exposure to acute/chronic copper, cadmium, DDT or nano toxic (nZnO). In general, we observed that chemical toxicity often increases with increasing temperature over the thermal tolerance range (TTR) of a species, and is further exacerbated at extreme temperatures (i.e., lower or higher than the TTR). Most of the aquatic organisms showed the highest tolerance to chemicals at their optimal temperature(s) where they displayed the highest value of median lethal or effect concentration. For aquatic animals, such universal phenomena can be well explained by the oxygen limited thermal tolerance theory explained by Hans Portner. Moreover, the overall temperature-dependent toxicity profiles vary considerably among different chemicals. Such differences may be partially attributable to the differences in temperature-mediated modifications of their physicochemical properties, toxicokinetics and bioavailability. For instance, we observed that ion dissolution of nZnO in seawater significantly increases with decreasing water temperatures. The diatoms exposed to nZnO had a significantly reduced growth rate at the lowest experimental temperature in contrast to the control; this response was probably due to the increased availability of toxic Zn ions at low temperatures. Recently, we have been conducting a novel meta-analysis to address whether the current source of AF10 (approx. 10) for fresh water quality guidelines (WQGs) would be sufficient to account for variation in chemical toxicity brought by thermal extremes. Our preliminary results suggest that AF10 seems adequately protective. Implications of our results will be discussed in relation to ecological risk assessments of chemical contaminants and derivation of WQGs for protecting aquatic life.

RA1A7-2

The calculation of risks due to mercury and other stressors to multiple endpoints at a regional scale for the South River and Upper Shenandoah River, Virginia USA.


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A cumulative integrated risk assessment has been performed for the South River from the area upstream of Waynesboro VA to the uppermost part of the Shenandoah River. The area is a site of historic mercury contamination from synthetic fiber production in Waynesboro. Six risk regions have been delineated. Other sources of other stressors include urban and agricultural run-off, channelization, erosion, and contaminated sediments and biota. The current iteration of the relative risk model (RRM) incorporating the above sources of stressors was applied. Risk regions, defined as having similar levels of risk (from highest to lowest) were delineated. Mercury is the stressor contributing the highest risk due to other stressors are large contributors. The endpoints at highest risk are those directly associated with ecological services. The Bayesian networks excellled at examining risks to specific endpoints while the RRM allows for gaps between endpoints. The risk assessment method was designed to be participatory with stakeholders in the study area.

RA1A7-3

Application of toxicological and ecological concepts to analyse multi stress in aquatic communities

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As a consequence of the growing human impact on ecosystems, freshwater organisms are often exposed to multiple stressors simultaneously, which can result in combined effects, leading to serious consequences for ecosystems. There is a need to develop a better understanding of interactive effects on ecosystems. Therefore, already existing concepts and tools in ecotoxicology and ecology have to be proofed for their validity and applicability in complex community responses to multiple stress. A microcosm study was conducted under controlled conditions and periphyton was used as test community. The effects of a resource stressor (saturated conductivity) and a toxic stressor (prometryn) were analyzed independently and both in combination. Structural (biomass, algal class and diatom composition, and functional parameters (tolerance development) were determined over a growth period of 6 weeks.

RA1A7-4

Responses of mean species traits in communities to multiple environmental stressors and the ecological risk assessment based on ecosystem function

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A trait-based analysis was conducted on a long-term (25 years) monitoring data of zooplankton community of Lake Kasumigaura, to elucidate relative importance of environmental stressor (temperature change, nutrient loadings, and chemical pollution) for the temporal changes in zooplankton community with respect to their contribution to an ecosystem function. I used the trophic transfer efficiency across three trophic levels as a measure of ecosystem function. Based on this measure, I identified species traits that were important for this function with a simple ecosystem model (the conversion efficiency of zooplankton was one of the most important traits). For the trait-based analysis, I made a database of traits (e.g. conversion efficiency, optimal temperature, range of suitable temperature, saprobic index, tolerance to chemical [carbaryl acute toxicity], median food size, and body mass) for major zooplankton species in Lake Kasumigaura. The long-term temporal changes of biomass-weighted mean traits in two trophic levels (May-September, and winter: October-April) were separately analyzed in conjunction with the environmental factors. The water temperature has been increasing at approximately 0.027 °C per year (climatic warming). There were long-term trends in traits: the mean body size and the mean tolerance to chemical had peaks on early 1990s but are decreasing in summer. In winter, however, they are increasing in recent two decades. The conversion efficiency is also increasing in summer but decreasing in winter. These observations suggest that the ecosystem function is severely deteriorated in winter. Similarities of temporal patterns between the functional traits and the environmental factors were examined with the Wavelet analysis. The results indicated that the zooplankton community synchronized clearly with water temperature in both seasons. The effect of inflated temperature was positive for the conversion efficiency in summer although this effect would be of conditional reduced chemical pollution because the temperature to chemical was highly correlated with the temperature preference of zooplankton.

RA1A7-5

Ranking the impacts of multiple environmental stressors on freshwater invertebrate and fish communities

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Achieving a good ecological status for waterbodies requires the identification of the relevant stressors to implement adequate measures. While the reduction of organic load resulted in acceptable low levels, restoration of the natural river morphology is now believed to be the most urgent task for water managers. Yet, several of these measures failed to rehabilitate the expected near-natural communities. At the same time, pesticides are frequently detected in surface waters that may limit the recolonisation of sensitive invertebrate species. The aim of the present study was therefore to discriminate between the effects of morphological degradation and pesticide stress on invertebrate communities. For this purpose, the SPEAR% index was introduced to identify the effects of habitat loss due to morphological degradation, which was not correlated to the other measures. To quantify habitat loss, relevant invertebrate variables available from field surveys were identified by PCA and combined to a overall habitat degradation score that was used for multiple regression modeling. To test if the pesticide input, the established run-off potential (RP) model was applied. Many of the classical metrics, such as the EPT Index or the German Fauna Index were highly interrelated and identified the predominant alkalinity gradient as major stressor. This was also the case for the SPEAR% index, which was expected to solely indicate pesticide stress. However, also the RP and the number of recolonization stretches were included in the best fit model of this metric, which had the overall best correlation of biological indices and environmental variables. The SPEAR% was not correlated to the other metrics and identified the depth as most important variable, although the correlation was not as strong as others. This correlation was even stronger for sites with low potential pesticide pollution, as indicated by high SPEAR% values and a low percentage of agriculture in the catchment. Our results suggest that pesticide stress has a similar or even higher impact on the ecological status than morphological degradation and that current-use degradation metrics are also influenced by pesticide stress. The latter may have important implications for future assessments of ecological status. Finally, the presence of recolonization stretches upstream alleviated the effects of pesticides in terms of higher SPEAR% values, which could be used as potential management option.
also being a significant factor (< 0.001), we suggest that exceptional future warming of eastern Australian coastline waters may limit the spawning season of key species.

We also note that fish can be robust to changes in pCO2 under clean water conditions, but that in combination with other stressors, such as temperature and/or pollution, changes in ocean physico-chemistry may pose a risk to continued recruitment. This study particularly highlights the importance of addressing the potential for interactive effects between climate change stressors and common marine pollutants.

RA17A-1
The importance of seasonal resolution to modelling the interaction of bioaccumulation and climate change
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From 16-21 July 2011 a SETAC Pellston workshop was convened to assess the influence of global climate change (GCC) on the scientific foundation and practice of environmental toxicology and chemistry. Workshop 1 focused on influences on chemical occurrence, fate and bioavailability. Here, I present our results for GCC impacts on bioaccumulation. These impacts occur through three primary mechanisms: influences on environmental exposure, on dietary exposure and on within-organism uptake and loss rates driven by bioenergetic processes. This work focuses on the bioenergetically-mediated impacts of GCC, building on previous modeling of species in the Laurentian Great Lakes.

A bioenergetics model for round goby (Apollonia melanostomus) was parameterized to reflect growth rates observed in Lake Erie, Laurentian Great Lakes. The impacts of climate change on bioenergetics was assessed based on a shift towards warmer annual lake surface temperatures. Simulations were run for the baseline case and for a 1, 2, and 3-degree Celsius increase in annual average temperature. The effects of this warming on chemical bioaccumulation were then estimated by coupling the bioenergetics model to a mechanistic bioaccumulation model for a broad range of hypothetical chemicals with log octanol-water partition coefficients (KOW) ranging from 0 to 8 and biotransformation half-lives ranging from 0.1 to 1000 days.

The impact of GCC on round goby growth illustrated the non-linear interaction between growth rate and fish thermal range. Two scenarios were chosen to showcase the impacts of GCC on bioaccumulation: the highest growth scenario, and the warmest scenario. When only annual average concentrations were considered, little difference among scenarios was evident. However, when the seasonal patterns of bioaccumulation were considered, substantial changes, both increasing and decreasing bioaccumulation, emerged. These seasonal impacts, which were more pronounced for metabolizable chemicals than for persistent ones, could be particularly important when they intersect with other time points, such as commercial fishing seasons or critical life stages for toxicological impact. The magnitude of the change from the baseline case depends most strongly on the biotransformation half-life, and then on KOW.

RA17A-2
Additive pressures from herbicides and elevated sea surface temperatures on symbiont-bearing foraminifera from the Great Barrier Reef
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Marine ecosystems are facing dramatic changes as a result of climate change. Changes in the physicochemical parameters of seawater systems, as a result of climate change, can potentially alter a number of factors that determine toxicity for any given pollutant. For marine systems, it is accepted that the world will contain warmer, more acidic oceanic conditions in the future changing the environment. These changes alone (increased temperature and/or decreased pH) have been shown to influence survival, development and reproduction for many marine species. However, these effects have been in uncontaminated waters. The reality is that many marine species will face the effects of seawater physicochemistry in combination with toxicant stress.

In order to better understand the combined effects of copper, elevated temperature and lowered pH on fertilisation success of an endemnic Australian sea urchin, Heliocidaris tuberculata, we present a study incorporating multiple stressors (3 temperatures x 3 pH x presence/absence of copper). The nominal copper concentration applied in these tests was based upon an EC50 calculated from five standardised toxicity bioassays. Potentiometric titration was performed to ensure pCO2 levels were maintained at conditions expected for eastern Australian coastal waters for the end of 2100 scenarios.

Results show that temperature and copper had a synergistic impact upon fertilisation, significantly (p < 0.05) reducing fertilisation success by > 50%. With temperature alone also < 0.001, we predict that exceptional future warming of eastern Australian coastal waters may limit the spawning season of H. tuberculata, which is already sensitive to high summer temperatures. Acidification, as a sole stressor, showed no significant effect on fertilisation (p=0.098). However, in combination with copper, low pH caused a significant decline in H. tuberculata fertilisation success (p < 0.001). As found in other studies, we conclude that sea urchin fertilisation may be most sensitive to changes in pCO2 under clean water conditions, but that in combination with other stressors, such as temperature and/or pollution, changes in ocean physico-chemistry may pose a risk to continued recruitment. This study particularly highlighted the importance of addressing the potential for interactive effects between climate change stressors and common marine pollutants.

RA17A-4
Evaluation of the combined action of natural stressors and chemical pollutants in algae. Assessment of functional, structural and metabolism alteration
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Nowadays, there is a growing number of studies exploring the combined effect of different stressors on ecosystems. However, the interactions between natural stressors and toxicants are still poorly understood. Among the stressors that might influence ecosystems, toxicants can directly or indirectly affect all relevant ecosystem processes such as primary production. On the other hand, fast and intense changes in the water temperature is one of the major threats for freshwater ecosystems. The objective of this study was to characterize the physiological responses of cultured algae, Scenedesmus vacuolatus in response to physical (temperature) and chemical (antimicrobial contaminants) stressors. The pollutants selected for this study were the priority pollutant diuron (herbicide, PSI inhibitor) and the emerging contaminants propranolol (β-blocker) and fluoxetine (antidepressant).

The experiment followed a factorial design with 2 factors (water temperature and toxicant concentration) and their interaction. A previous experiment determined that the optimal temperature was 20°C, while 30°C was used for simulating physical stress. Chemical stress was reproduced at the level of EC30 for each contaminant (5, 850 and 500 µg/L for diuron, propranolol and fluoxetine, respectively). Changes in photosynthetic efficiency (Yef), photosynthetic capacity (Ymax), photosynthetic quantum (pQ) and non-photochemical quenching (qP) were studied at 30°C and exposed algal cultures. The algal toxicity of the three compounds differed considerably. Diuron was the most toxic compound, followed by fluoxetine and propranolol. Effects of diuron occurred 135

SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting
Chemical exposure enhances outbreak of infectious disease in fish

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Heavy oil (HO) pollution is one of the most important environmental issues in the world. In our previous study, we evaluated immunotoxic effects of HO on Japanese flounder (Paralichthys olivaceus), and found that 0.3 g/L of HO led immune suppression at cellular and molecular levels in the fish. Moreover, in the experimental infection with viral hemagogic septicaemia virus (VHSV) to the fish exposed to HO, we obtained higher mortalities in dual stressor group (virus infection with HO exposure) than those in control groups. In this study, we investigated the mechanisms of disease occurrence in the fish given the dual stressor by microarray experiment and dynamic of viral replication in the host fish. After applying stress to the fish by each single stressor or by the dual stressor, the mortalities of the groups were calculated and the fish were dissected for sampling of kidney for the microarray experiment and heart for virus titration. As the results, fifty percent of the fish died in the dual group, while no mortality was observed in single stressor groups as well as in control. These results indicated that the dual stressor induced lethal effect in the fish, even when each single stressor had no effect. To investigate if the mortality in the dual group attributed to viral hemagogic septicaemia (VHS), we measured the virus titre in the heart sample from each group. The infectivities per g heart tissue were higher in dual group (102 to 108.25 TCID50/g) than those in VHSV group (103 to 106.8 TCID50/g). This suggests that VHSV easily replicated in the host fish in the dual stressors and caused a death in the VHSV group.

RA17B-6
Interactive mixture toxicity effects of a cyanobacterial stressor and insecticides may partly be grouped according to insect mode of action

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We investigated mixture toxicity of a harmful cyanobacteria (i.e., Microcystis aeruginosa) and insecticides with different modes of action to Daphnia pulex. The widespread occurrence of such toxic cyanobacterial blooms has become an important concern for aquatic ecosystems. In agricultural areas, these toxins may act in combination with plant protection products, including insecticides. In order to study such combined effects, we exposed the waterflea Daphnia pulex to binary mixture combinations of Microcystis and 8 insecticides for a period of 21 days according to a modified closed system design. Results were statistically analyzed with the concentration addition and independent action reference models to test for additive, synergistic or antagonistic mixture toxicity. Synergistic effects were observed on reproduction for the insecticides lindane and M. aeruginosa while fenoxycarb, imidacloprid and spinosad caused synergistic effects on length in combined with M. aeruginosa. Linking the results with the mode of action, we observe no interactive effects in combinations with insecticides affecting the acetylcholine pathway by inhibition (carbaryl and chlorpyrifos). However, synergistic effects on daphnia size are observed with those insecticides that affect the acetylcholine pathway by agonistic or allosteric activity (imidacloprid and spinosad). Although endosulfan has a different molecular target compared with imidacloprid and spinosad, both of these receptors belong to the same superfamily of Cys-loop ligand-gated ion channels. This could explain the common observation of synergistic effects in all combinations with these three insecticides. Combination of tebufenpyrad and M. aeruginosa resulted in antagonistic effects on both length and reproduction. Interestingly, both can affect the oxidative phosphorylation through completely different mechanisms. Tebufenpyrad specifically inhibits electron transport in mitochondrial complex I while Microcystis is known to affect the oxidative phosphorylation superfamily of Cys-loop ligand-gated ion channels. This could explain the common observation of synergistic effects in all combinations with these three insecticides.

RA18-1
Risk of severe oil spills - was deep water horizon an outlier?

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Following the explosion of the drill rig Deep Water Horizon (DWH) on April 20, 2010 that killed eleven workers, an estimated 670000 tons of oil were spilled in the Gulf of Mexico until the well could be capped on July 15th. This makes DWH the largest single unintentional spill in the history of drilling for oil.

Based on global data of oil spills since 1974, we estimate the expected return frequencies of such very severe oil spill events for different spill sources through the oil chain to answer the question if the DWH spill can be considered an outlier.

This is particularly important in view of the rapid increase in deep and ultra-deep offshore activities, where both a geographical expansion as well as a trend towards drilling at ever greater depths can be seen over the last decade.

We also compare the risk of oil spills from offshore drilling with the risk of spills that are posed throughout the entire oil chain, separately for different infrastructures such as pipelines, tanker ship transport and storage. Data is extracted from our uniquely comprehensive global Energy Related Severe Accident database (ENSAD) that contains accident data from a large number of different sources. The severity is modeled with a generalized Pareto distribution, to measure specifically the risk of very severe accidents.

The results give a mean return frequency based on historical data since 1974 of spills from offshore platforms and rigs exceeding the 670000 tons of the of the Deep Water Horizon oil spill of around 19 years with 5% and 95% quantiles of 7 years and 49 years respectively. Based on this result this outlier cannot be considered an outlier.

RA18-2
Where has all the oil gone? Identification and toxicity of oil degradation products

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Oil is a highly complex mixture containing hundreds of thousands of components. Recent analyses using two-dimensional gas-chromatography mass spectrometry (GCxGC-MS) of the acid-extractable fraction of oil sands process-affected waters (OSPW) from Alberta Canada has shown that even hydrocarbons thought to be extremely resistant to biodegradation could be biodegraded. Some of these so-called 'naphthenic acids' (NA) also have also been identified in extracts derived from crude oils and therefore likely also occur in the environment as a result of degradation of oil following accidental spillage. Previously we have reported quantitative structure-activity relationships for several structural groups of individual NA using a standard microbial toxicity assay. Now we present the toxicity of individual NA when combined as mixtures. For oil-industry produced waters, marine species may be exposed to these acids. We have now tested the effects of acute exposures to three commercial preparations of NA (CNA) on marine mussels. Many NA are not available in sufficient quantities for toxicity testing. Consequently, we have modelled the toxicity of over 50 acids for a large number of environmental endpoints (e.g. fathead minnow lethality) and an array of human health measures such as endocrine disruption.

Structural class mixtures of individual NA plus a 35-component mixture was tested using the Microtox® assay. Mytilus galloprovincialis, were exposed to oil with different concentrations. Mussels were exposed to a series of decreasing concentrations, from 0.3 g/L of HO led immune suppression at cellular and molecular levels in the fish. Moreover, in the experimental infection with viral hemagogic septicaemia virus (VHSV) to the fish exposed to HO, we obtained higher mortalities in dual stressor group (virus infection with HO exposure) than those in control groups. In this study, we investigated the mechanisms of disease occurrence in the fish given the dual stressor by microarray experiment and dynamic of viral replication in the host fish. After applying stress to the fish by each single stressor or by the dual stressor, the mortalities of the groups were calculated and the fish were dissected for sampling of kidney for the microarray experiment and heart for virus titration. As the results, fifty percent of the fish died in the dual group, while no mortality was observed in single stressor groups as well as in control. These results indicated that the dual stressor induced lethal effect in the fish, even when each single stressor had no effect. To investigate if the mortality in the dual group attributed to viral hemagogic septicaemia (VHS), we measured the virus titre in the heart sample from each group. The infectivities per g heart tissue were higher in dual group (102 to 108.25 TCID50/g) than those in VHSV group (103 to 106.8 TCID50/g). This suggests that VHSV easily replicated in the host fish in the dual stressors and caused a death in the VHSV group. From the results of microarray experiment, the expressions of antiviral activity related genes such as interferon and apoptosis induction were relatively lower in the dual group compared with those of VHSV infection group. These results supported the high virus titre in the fish given the dual stressor. In conclusion, interferon production in the virus-infected cells and apoptosis induction by NK cells worked in a normal manner in the VHSV-infected fish without HO exposure, but the antiviral activities were suppressed in the fish affected by the dual stressor, which might lead to extensive viral replication in the host cells, resulting in the occurrence of VHS.

Use of ecosystem service valuation in quantifying ecological impacts and compensatory restoration associated with oil spills in the environment

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Since the Exxon Valdez spill, approaches to quantify the potential impacts of an oil spill on the environment have evolved significantly. These approaches were derived out of the need to make the public whole for impacts to the environment. The approaches evolved from a strict monetary compensation framework to an ecosystem service based compensation process. That is, given that there was an impact on the environment, impacts to ecosystem services (ecological and human use services) were to be quantified and then, based upon the lost ecosystem services, the public was to be compensated by the provision of an equivalent amount of ecosystem services through the
implementation of site restoration projects. As such, the compensation (restoration) was scaled to the level of injury. This overall approach is termed the service-to-service or damage assessment.

**RA1-8**

Effects of chemically and mechanically dispersed oil on fitness-related and molecular endpoints in the North Atlantic copepod Calanus finmarchicus


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In recent years there has been an increasing emphasis on the significance of invertebrates for assessing environmental impact of oil spills. In the event of accidental oil spills in sub-Arctic and Arctic marine environments planktonic organisms like copepods are realistic targets for oil toxicity based on their significant role in the food web, their abundance and their large lipid content. For many years the SINTEF/NTNU culture of Calanus finmarchicus has functioned as relevant model for standard ecotoxicity testing of North Atlantic crude oils, and a large database of ecotoxicity data exists for this species. Parameterized experimental data on the effects of oil (single oil components, water soluble fraction of oil, and dispersed oil) on copepod survival and reproduction are used as input for development of numerical models for environmental risk and damage assessment. The accessibility of a continuous copepod culture provides homogeneous specimen in terms of developmental stage and lipid content. This, along with sophisticated experimental systems, is a major factor facilitating research on ecotoxicity testing of dispersed crude oil, based on 260,000 ESTs sequenced using FLX454 technologies. Several methods, like 1H-nuclear magnetic resonance and mass spectrometry, have also been developed and applied in order to investigate metabolic profiles and alterations. Together these complementary methods give valuable supporting information to well known fitness-related endpoints, as they contribute with modes of toxic action of stressors, and output data may also be used to determine effect limits. The presentation will include results from an environment aimed at comparing the effects of chemically and mechanically dispersed oil, their modes of toxic action, and proposed effect limits of toxicity based on fitness-related endpoints as well as molecular profiling. These data will provide input to environmental models for risk and damage assessment following acute oil spills.

**RA1-8**

Temperate and polar marine species sensitivity to oil components in relation to accumulation kinetics

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Risk assessments for polar marine ecosystems are mostly based on toxicity data obtained for temperate species. Yet, it is unclear whether toxicity data of temperate organisms can be used to derive reference values for protection of polar species, as differences in physiological characteristics, like metabolism and lipid composition, may yield different results for toxicants. The first aim of our study was therefore to compare polar and temperate marine species on their sensitivity to oil. To that end, species sensitivity distributions (SSDs) were constructed for crude oil, 2-methyl-naphthalene, and naphthalene based on acute toxicity data from scientific literature and databases. To allow for an estimation of the overall risk of oil contamination in the field, toxicity thresholds of oil components are needed. Therefore, our second aim was to model oil toxicity and transformation of oil fractions in marine organisms, to evaluate the outcome of model calculations and to compare with field data. The molar concentration for 50% of the organisms (LC50) was calculated using a critical body residue for compounds acting by narcosis and a weighted average of log octanol-water partition ratios (Kow) of the components constituting oil. The LC50 value is related to the concentration of oil components and is estimated LC50 value for naphthalene, 3.0·103 µg/l and 5.7·103 µg/l, respectively, showed little difference. Therefore, the average toxicity of naphthalene to temperate marine species can be predicted based on accumulation kinetics. A Kow of 105 and an octanol-molecular mass of 200 yielded an LC50 of 2·103 µg/l for oil in general. A more refined calculation taking into account biotransformation and specific modes of action underpinning this value.

**RA1-8**

The sensitivity of polar and temperate marine species to oil and oil components differed on average less than a factor of 3. In addition, most of the differences were not statistically significant and there was no taxonomic group that was consistently more sensitive than the other groups. Apparently, physiological mechanisms suggested to cause differences between polar and temperate species have little overall effect on sensitivity to oil. As a consequence, toxicity data obtained for temperate organisms may serve as a good indication for the first indication of the risks in polar regions. Yet, exceptions may result from biotransformation and specific modes of oil action.

**RA1-8**

Integrating marine physics, biological and eco-toxicological models into a unified simulation system for oil spill risk and impact assessment

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A 3-year project called SYMOBIOSE has been initiated to develop a holistic, integrated modelling framework for ecosystem-based risk and impact assessments. The strategy is to create a continuously evolving numerical model, each of which has been previously developed, validated, and proven useful. This approach avoids the cost of basic code development and allows for the different challenges in that the various components are based on quite different numerical processes. The system consists of physics, biological, oil/chemical fate and eco-toxicological components. The physics models are Eulerian, as are some of the biological models, whereas the pollutant fate and some of the biological components are Lagrangian. The related process equations of the component models are solved in general on different time-steps, and at different spatial resolutions. The design of the system requires the possibility of two-way communication between model components (e.g. zooplankton feeding on phytoplankton, zooplankton growth and reproduction of appropriate bacterial taxa, and processing growth of phytoplankton, mortality, growth and reproduction of zooplankton, and growth and mortality of ichthyoplankton). It is also desirable that alternate components can be inserted into the system, to facilitate geographic transportability as well as uncertainty analyses. We therefore seek a relatively flexible and transparent set of methods to achieve integration of the separate models into the system. We assume that the physics models are always Eulerian: regardless of numerical solution, the computations are carried out on a regular or irregular grid that is spatially fixed for the duration of a given simulation. The physical and oil/chemical transport and fate models may be either grid-based or particle-based (pseudo-Lagrangian), and will in general produce data on spatial scales different from that of the physical environment models. This paper will describe the proposed design plan to meet these challenges.

**RA1-9**

Plants and chemicals in the environment: risk assessment, pest management and phytoremediation


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**RA1-9**

Risk assessment of herbicides for the common buttercup Ranunculus acris in field margins - an experimental field study

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Field margins comprise the majority of semi-natural habitats in the intensively farmed agricultural landscape and thus can benefit the conservation of biodiversity in agroecosystems. However, field margins can be negatively affected by pesticide by direct overspray and spray drift from field applications. The risk assessments of herbicides are often performed in simplified simulations or field trials and annual plants are often seen as the first development stages in greenhouse experiments. But the vegetation of field margins usually consists of annual and perennial plant species in different development stages. Also insufficient knowledge about the sublethal and long term effects of herbicides on plants is available.

The present perennial field study (start 2010), was undertaken to investigate the effects of repeated herbicide applications in successive growing seasons on Ranunculus acris in field margins. The test design followed a randomized block design (7 treatments, 1 control, 8 replicates). The applications of the treatments and their application sequences mimic the field management of winter wheat fields with their recommended agrochemical products and application rates. The applied fertiliser and pesticide concentrations
are consistent with their inputs (drift/overspray) in the first meter of a field margin directly adjacent to a field under Good Agricultural Practices.

To detect the effects of the applications vegetation assessments and a photo-documentation of the flower intensity of 

RA1-2  Enhancing risk assessment by using a toxicokinetic and toxicodynamic (TK/TD) growth model of Myriophyllum spicatum

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Toxicological studies used for risk assessment can only cover a limited range of exposure scenarios due to their work intensity. Ecological models considering the toxicokinetic and toxicodynamic of chemicals are capable to close the lack of exposure scenarios in toxicological studies and, thus, enhance risk assessments by predicting the effects of variable exposure scenarios.

In this work a toxicokinetic and toxicodynamic growth model of Myriophyllum spicatum is presented giving the ability to predict the effects of chemical substances on the growth of M. spicatum. Therefore, a growth model considering the most important factors influencing the growth was developed. A toxicokinetic part calculating the uptake and distribution of chemicals depending on their physicochemical properties and the physiology of M. spicatum was included in the growth model. Moreover, a toxicodynamic part using the internal concentration in M. spicatum and experimentally established dose-response relationships to modulate the growth rate of M. spicatum was added to the model. The model is able to predict reversible growth inhibition under different environmental and exposure conditions based on standard test results.

The model was verified with experimental data on growth inhibition of M. spicatum after fourteen days due to different concentrations of 3,5-dichlorophenol (DCP). The model was able to predict the effect of 3,5-DCP exposure on M. spicatum very well but cannot fully explain the total inter experiment variability of growth, particularly under untreated conditions. The model can be used to predict growth inhibition for 3,5-DCP. Further validation and verification of the model is needed to ensure that the model works properly and to show that the model can be used for a wide range of substances with different physico-chemical properties.

RA1-3  Herbicide impacts on macrophytes: can we predict community-wide effects from single-species toxicity tests?

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RA1-4  Linking aquatic plant toxicity data for pesticides to risk assessment endpoints and environmental protection goals

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This presentation discusses protection goals for aquatic plants, assessment endpoints that address those protection goals, and the relationship of standard toxicity data to the assessment endpoints and protection goals. Protection goals for aquatic plants generally focus on the plant community as a whole, rather than particular species or individuals as is the case for aquatic animals. Consistent with these protection goals, it is not necessary to completely protect every sensitive plant species; protecting some fraction of plant species (represented by a certain percentile of the Species Sensitivity Distribution, SSD) is sufficient to protect overall community function and structure. Assessment endpoints used to characterize effects of chemicals on aquatic plants should represent impacts of similar severities to assessment endpoints used for animals, in relation to their respective protection goals. Toxic endpoints for aquatic plants are based on non-lethal responses, unlike acute endpoints for animals which are based on mortality.

Furthermore, aquatic plant communities usually recover more quickly than animal populations (especially fish) from effects of stressors. These considerations suggest that assessment endpoints for aquatic plants should be selected to higher SSD percentiles than the 5% typically used for animals. When data are unavailable for a sufficient number of species for SSD analysis, a small number of surrogate test species (e.g. Lemma gibba, Myriophyllum spicatum, and certain algae) can indicate the toxicity of herbicides and fungicides to the most sensitive aquatic plants.

RA1-5  Uptake and intra-cellular accumulation of hydrophobic chemicals in charophytes and implications for ecosystem exposure control and remediation

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Uptake to primary producers (constituting an important pool of organic carbon in lakes) is a key step for addressing hydrophobic chemicals to upper trophic levels. It has been hypothesized that permeation and diffusion through biota surface structures such as epitelia, cell walls or membranes may be inhibited for highly hydrophobic substances by steric hindrance of membrane passage. Chara rudis is a macroscopic, perennial, benthic taxon having a protective layer of cortex cells. We used 14C12 radiolabelled Hexachlorobenzene (HCB) to i) investigate whether or not HCB can reach the internode cell, ii) to assess the distribution of HCB in different plant parts, and iii) to discuss the implications of the accumulation on benthic macroalgae for fresh water ecosystems. We found that the chemical was almost fully associated to the algae tissues, the HCB in the cortex cells represented about 90 to 95% of the total found in the plant, and HCB was detected at measurable levels in 57% of the sampled internode cell cytoplasm, demonstrating the occurrence of intracellular transport and storage of chemicals. In some water bodies charophytes grow in very dense meadows up to 2m tall and can cover a large fraction of the water body bottom. The high efficiency of taking up hydrophobic chemicals directly from the water phase suggests that they can also represent a key control for the mass balance of POPs in the water ecosystem wherever they are abundant.

RA1-6  Halophyte filters: the potential of using halophyte species for phytoremediation purposes in saline aquaculture

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There is a growing consumer demand for seafood as protein source, and land-based (marine) aquaculture is seen as a sustainable way to meet this growing demand. A major problem with aquaculture is the nutrient waste, since most of the nutrients added through feed are released into the environment, predominantly in dissolved form. Filtration and sedimentation techniques to reduce nutrient concentrations are not adequate for the large volumes of waste water produced in aquaculture. The use of constructed wetlands has been shown to be successful in freshwater aquaculture practices. Freshwater constructed wetlands are worldwide used to treat various types of wastes. However, there is only limited experience in saline systems. The main aim of this study is to analyse the potential of constructed saline wetlands in land-based marine aquaculture. The main advantage of using wetlands is that these are relatively simple systems that need little control after construction. The location of the wetland can be located close to the source, limiting transport of waste water through pipelines. Further, wetlands can simultaneously reduce several contaminants (BOD, suspended solids, nutrients, pesticides, pathogens). The primary function of a constructed wetland is the purification of water, but there are also several ancillary benefits that can be incorporated in wetland treatment designs. For example a high vegetation biodiversity, offering a habitat for fauna, and giving aesthetic, recreational, commercial, and educational human uses. Different approaches exist to utilize plants (halophytes, macro-algae, micro-algae) in the treatment of marine aquaculture effluent; these are described in a conceptual framework. In essence, the approaches attempt to maximize the ecosystem service of water purification. The approaches differ in the balance between economic benefits and nature benefits. The potential use of this framework is demonstrated with a Dutch case study.

RA2-0  Risk assessment of chemical mixtures: where do we stand? what are the next steps?

RA2-1  Predictive regulatory risk assessment of chemical mixtures in the aquatic environment: a conceptual framework

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Risks of chemicals in the aquatic environment are still often assessed substance-by-substance, neglecting mixture effects. This may result in risk underestimations, as the typical exposure is towards multi-component chemical "cocktails". We used the two well established mixture toxicity concepts of concentration addition (CA) and independent action (IA) for developing a tiered scheme for environmental hazard and risk assessments of mixtures, focusing on general industrial chemicals regulated in the EU under REACH and assuming that the so-called "base set" of toxicity data is available, i.e. EC50 values for algae, crustaceans, and fish. As mixture toxicities higher than predicted by CA are rare findings, we suggest applying CA as a precautionary first-tier - irrespective of the modes of action of the mixture.
components. In particular, we show that summing up PEC/PNEC ratios might serve as a justifiable CA-approximation, in order to extrapolate from the "base set" data to the aquatic ecosystem in a regulatory first tier assessment. This approach makes optimum use of already existing single substance assessments. More in-depth mixture investigations may be requested only if the first tier estimates give an indication of a potential environmental risk. Finally we suggest to call for mode-of-action driven analyses only if error estimations indicate the possibility for substantial differences between CA- and IA-based assessments.

**RA2-0**

**Bearing down the borders? - Considerations on an environmental risk assessment of substance combinations across different regulations**


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Across Europe, the prospective environmental risk assessment (ERA) of chemical substances is conducted under separate regulatory frameworks, i.e. for plant protection products, biocides, industrial chemicals as well as human and veterinary pharmaceuticals. The main conclusion of this assessment is to avoid adverse effects of these chemicals a priori to an exposure of the environment. Under all regulations, the current assessment methods focus on single substances only. As it is well accepted that multiple substances typically reach environmental compartments together and act jointly on organisms, strategies and methods for an assessment and regulation of chemical mixtures are currently under development for all these regulatory frameworks. The presentation focuses on the activities at the “Chemical and Biological Safety” Division of the German Federal Environment Agency (Umweltbundesamt, UBA) with a focus on the development of common methods and strategies for the consideration of substance combinations under the different legislations. Furthermore the limitations and needs for an assessment of mixtures that reach the environment from multiple sources, i.e. substances that traditionally fall under different legislations, are pointed out. Existing approaches for overarching concepts beyond substance-oriented regulations are discussed from an regulatory perception. Common agreements on definitions, assessment methods and strategies across the substance-oriented regulations are important. The same applies for an exchange of knowledge and data between regulations, which would enable an assessment of substances from a variety of sources. Overarching concepts might be helpful for certain situations and substances, but it needs to be clarified for which cases and who might conduct such an assessment.

**RA2-3**

The threshold of (eco)toxicological concern: a suitable tool for mixture risk assessment and ranking?

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The threshold of toxicological concern is defined as a safe level: a concentration at or below which there is no appreciable risk for humans (TTC) or the environment (ecoTTC). Recently, the TTC concept has also been put forward as a tool for the risk assessment and ranking of chemical mixtures, for example in the recent opinion on mixture toxicity assessment by the scientific committees of the European Union. In particular it has been argued that compounds that are present at or below their individual (eco)TTC do not contribute to the (eco)toxicity of a mixture. That is, a mixture would pose no risk for human health or the environment, as long as all components are present only in concentrations at or below their individual (eco)TTC. The TTC approach has a range of appealing features. It would be extremely helpful for simplifying the (eco)toxicological assessment of complex mixtures by allowing to ignore compounds below their individual (eco)TTC. It would also simplify the problem of mixture toxicity assessment to a single substance assessment, as we can safeguard against any mixture effect, as long as we can ensure that the concentrations of all compounds never exceed their individual (eco)TTC. Furthermore, the (eco)TTC seems to provide a good basis for a risk-based weighing and exposure-based weighing of each substance in the mixture. The TTC approach is currently developed for the purpose of mixture toxicity assessment in the context of e.g. REACH. A first ecoTTC-like approach is already implemented in the form of the so-called action limit in the European guideline for the environmental risk assessment of pharmaceuticals.

I will briefly review the conceptual basis of the (eco)TTC, the suggested applications in the context of mixture toxicity assessment and will then discuss the implications of its application in view of the classical mixture toxicity concepts (Concentration Addition and Independent Action), which are the cornerstones of our current understanding of mixture (eco)toxicology. The main conclusions are that (i) the (eco)TTC concept requires constant update of the underlying (eco)toxicological data, as the chemicals in use change over time, (ii) the (eco)TTC concept needs to be adjusted for mixtures that contain at least partly compounds with a similar mode of action, which might make it primarily useful for risk management, and (iii) that in particular the ecoTTC requires further development and refinement if it is to be used in the context of ecological protection goals.

**RA2-4**

Long-term trends in potential toxicity of unknown organic micro-pollutants in rivers

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During these years, the effects of toxic substances on the ecosystem in Dutch inland waters were measured with a complementary method, i.e., by means of so-called bioassays. This approach provides information on the effects of unknown chemicals in water which are overlooked by traditional analytical techniques. The latter cover only a small portion of the large number of chemicals that are present in surface water. Moreover, classical chemical techniques do not give insight into the auxiliary effect that several toxic substances may have.

The results from the bioassays confirm that damage to the aquatic ecosystem during the last decade due to the presence of toxic substances has decreased. Toxic pressure in water of the river Meuse and Scheldt was significantly higher than that in the river Rhine, but has decreased considerably since the year 2000. The results also indicate that the toxic pressure is higher upstream and decreases downstream. The reaction of five organisms to toxic chemicals in a water sample was measured with bioassays. Applying the species sensitivity distribution method to this small set of data results in a snapshot of the toxic stress. This approach is however flawed by large uncertainty margins which make a series of snapshots unsuitable for discerning a trend in water quality. A trend became apparent when all bioassay results collected over the whole period were combined by means of an advanced statistical technique. As a result, information on toxic trends becomes more accurate because the multitude of data has reduced the spread in toxic stress in river water sampled at a given river bank location. Responses to the bioassays provided insight into the nature of the toxic compounds. The cocktail of toxic substances in the river Rhine was found to consist of non-polar chemicals, i.e., substances without a specific mode of action which affect all aquatic organisms. In the other rivers, pesticides are probably responsible for the observed effects.

In the summer of 2002, the river Meuse must have been polluted by both known (albeit ban for more than ten years at that time) and unknown herbicides, as revealed by a comparison of chemical measurement and bioassay results.

**RA2-5**

Toxicity of metal mixtures to Daphnia magna: Implications for a multi-metal, multi-site biotic ligand model


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In real-world aquatic systems, organisms are usually exposed to metal mixtures instead of individual metals. To predict the toxicity of metal mixtures, we have been developing a mechanistic model based on tissue residues of metals and on the concept that the toxicity of a mixture of metals can be either dose-additive or response-additive, depending on the mechanisms of action. To calculate tissue residues and thereby predict toxicity across wide ranges of water quality, we have been developing a multi-metal, multi-site biotic ligand model (MMMS BLM) that concurrently accounts for metal-metal competition for binding on dissolved ligands in the water and at sites of toxicity on organisms. We have used Daphnia magna to mixtures of Cu and Zn, Cd and Cu, or Cd and Zn in moderately hard reconstituted water containing dissolved organic matter (added as Suwannee River fulvic acid) at 1 mg DOC/L, and compared observed mortality to the null assumption of additive mortality predicted from results of concurrent Cd-only, Cu-only, and/or Zn-only toxicity tests. This research has revealed several apparent metal-metal interactions that otherwise might lead to conclusions that metals interact in non-additive ways, yet simple geochemical speciation in the BLM can explain these interactions and reconcile the apparent non-additive toxicity. For example, the toxicity of Cu-Zn mixtures always appeared to be more-than-additive or additive when based on dissolved metal concentrations, whereas Cu was varied while Zn was held constant. Conversely, Cu-Zn mixtures always appeared to be less-than-additive or additive when based on dissolved metal concentrations. These results demonstrate that different metal mixtures can appear to interact differently based on dissolved metal or free-ion concentrations.
address diagnostic, mechanistic or extrapolation questions. Since 2002 almost 40 studies were published with their major focus on mixture toxicity assessment by means of toxicogenomic techniques, mainly through microarray or qPCR techniques, though metabolic and proteomic analysis of joint exposures have also been undertaken. It is now standard to explicitly state criteria for selected concentrations and provide insight into employed data transformation, and statistical treatment with respect to minimising sources of undue variation.

The datasets used may differ among the frameworks, not only because of different ways of literature searching, but also because of diverging choices made in assessing reliability and relevance. The use of outbred laboratory animal strains representing wild populations is often advocated but rarely demonstrated in ecotoxicology. Due to practical constraints limiting the use of outbred strains, and the need to have animal models more closely resembling the target species, the use of wild-derived strains has become more common. However, wild-derived strains are often less reliable and relevant than inbred strains.

For EQS derivation according to the draft guideline of the EU, the use of wild-derived strains is not required. However, the use of wild-derived strains is highly recommended for risk assessment purposes. This is because the use of wild-derived strains can provide more realistic information on the effects of chemicals on populations. The use of wild-derived strains can also help to reduce the number of animals used in toxicity tests.

RA21-1 - Standard vs non-standard methods for hazard and risk assessment

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The use of public literature differs among the various frameworks, partly because of the specific guidelines but also because public literature cannot always be assessed for its reliability, the scores of Klimisch [2] are used, with a division into four categories: 1 = reliable; 2 = reliable with restrictions; 3 = unreliable; and 4 = unassignable.

The use of public literature in the derivation of risk limits, e.g., PNECs, in REACH and the framework of plant protection products is reviewed. For EQS derivation according to the draft guideline of the WFD, all relevant available information should be considered. This means that dossier data submitted under the relevant frameworks should be used, but also data from open literature should be included, provided that the scientifi c reliability is sufficient and endpoints are relevant. For reliability assessments [2] are used, with a division into four categories: 1 = reliable; 2 = reliable with restrictions; 3 = unreliable; and 4 = unassignable. Only studies with a validity score of 1 or 2 can be used for EQS derivation. However, not all valid studies are also relevant for EQS derivation. Only endpoints which are relevant to the population should be taken into account. Thus, endpoints like histopathology, blood parameters, general activity, swimming speed, organ weight and results from in vitro tests cannot be used for EQS derivation, even if this would result in more critical values.

RA21-2 - Improved protocols for sediment toxicity testing: a review

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RA21-3 - Use of public literature and dossier data in WFD EQS derivation compared to risk limit derivation in other regulatory frameworks


In the Netherlands, RIVM has a broad experience on the derivation of Environmental Quality Standards (EQSs) under the Water Framework Directive (WFD) and the evaluation of test data within this framework. An EQS derivation, which will then be compared to the use of public literature in the derivation of risk limits, e.g., PNECs, in REACH and the framework of plant protection products.

RA21-4 - Standard and non-standard ecotoxicity tests in regulatory risk assessments of chemicals

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Guidance documents recommend the use of standard ecotoxicity tests in regulatory risk assessments [1-6]. These recommendations have decreased the use of non-standard test methods for several groups of chemicals. As ways forward we suggest to study and establish quantitative relationships between dose dependency and time dependency of responses.
documents recommend that the method described by Klimisch et al. [9] should be used for evaluating the reliability of ecotoxicity and toxicity data but the Klimisch criteria give a strong preference for standard tests.

We present a novel and more comprehensive method for evaluating and reporting non-standard ecotoxicity data [10]. Its aim is to enable an increased use of non-standard data in risk assessments. As part of this work we clarify the definitions of "reliability" and "relevance" in order to promote the consistent and application of these concepts in risk assessment procedures. Lastly we present examples from environmental risk assessments of pharmaceuticals showing how non-standard data can complement standard data to arrive at robust and transparent risk assessments.

RA21-5
Toxicity and detoxification of chemicals in detergents, softeners and shampoos
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Recently environmental concern was mainly focused on the intentional release of chemicals from use of pesticides and discharges from industries. Presently concern has also been raised on non-intentional release of chemicals from articles and products like paints, textiles, tires, plastics, pharmaceuticals, and personal care and cleaning products. For all chemicals their hazard and risk is based on toxicity (including genotoxicity and senescence), degradation and biocumulation, either from real testing or chemometric modelling. However, for products and articles, which may contain many chemicals at confidential concentrations, assessments of biodegradation, biocumulation and combined toxicity based on ingredient toxicity are not possible to make. Therefore, an approach similar to that used for industrial wastewaters using toxicity testing and, when necessary, TIE (Toxicity Identification Evaluation) might be used. Since many chemicals will reach the environment via sewage treatment works, their biodegradation and detoxification are important for their environmental ecotoxicity. Research on detergents, softeners and shampoos has shown that surfactants are key chemicals for the toxicity of these products, and that there is a wide range in product toxicity, as well as in their detoxification. Recent studies, using the standard ISO test with Daphnia (ISO 6341) and the acute toxicity (48 h immobility test) with Hyperia salina (HFFRs) that are already commercially available, have demonstrated that ATO, APP and ZHS did not show high aquatic toxicity. Also, resistance to anticoagulant rodenticides (ARs) are non-specific in their toxicity and so liver residues have been measured in non-target species to gain information on scale of exposure and to assess the likelihood of effects. The second-generation anticoagulant rodenticides (SGARs) have been a focus for monitoring because their widespread use, high acute toxicity and persistence enhance potential for secondary exposure and poisoning. We review what monitoring has told us about the key factors that mediate exposure of non-target species to SGARs, and discuss the importance of resistance in mediating exposure and risk.

To determine the EC50 values, the compounds were subjected to 48 h immobility tests with Daphnia magna, based on OECD guideline 202. For each compound, first the concentration that equals the maximal water solubility (max. Sw) was tested. Second, if an effect was observed at max. Sw, a dilution range was prepared (4 concentrations per compound) and tested to determine the EC50. The alternative flame retardants studied included six organic phosphates (Aluminium Diethyl Phosphinate (ALPI), Bisphenol Pentaerythritol Triethyl Phosphate (TPP) and six inorganic compounds (Aluminium Trihydroxide (ATH), Ammonium Polyphosphate (APP), Antimony Trioxide (ATO), Magnesium Hydroxide (Mg(OH)2) and ZHS). A modelling approach was used to study the transference of the ARs into the environment during AR treatments for Norway rat control. Baiting with brodifacoum resulted in lower levels of AR entering the food chain via the rats and lower numbers of live rats carrying residues of AR during and after the trials due to its effectiveness against resistant rats. Bromadiolone and difenacoum resulted in markedly higher levels of AR uptake into the rat population and more live rats carrying residues during the trials and for long periods after the baiting period. Neither of these compounds provided full control on any of the trial farms. Secondary non-target predators were predicted to take up more AR when residues in rats were higher and the more rats remained alive. In resistant areas where ineffective resistance influences the total amount of AR available to non-targets and should be considered when dealing with rat infestations, as resistance-breakers may present a lower risk to wildlife.

RA22-2
What do anticoagulant rodenticide residues in predatory birds and mammals tell us about non-target exposure and risk?
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Anticoagulant rodenticides (ARs) are non-specific in their toxicity and so liver residues have been measured in non-target species to gain information on scale of exposure and to assess the likelihood of effects. Exposure of predatory birds and mammals to SGARs is widespread but species vary in their accumulation of liver residues. Diet is assumed [but rarely shown] to be a major factor yet the differences in residue accumulation occur between species with similar diets. However, a recent study strongly suggests that diet can indeed be a key factor. When prey guild is restricted, foxes (Vulpes vulpes) feed relatively extensively on commensal rodents and other species likely to take AR bait. As a result, they accumulate greater SGAR residues than animals from areas where prey choice is wider and includes species unlikely to encounter bait. Usage is also likely to influence exposure. At large spatial scales, the overall pattern of wildlife exposure reflects SGAR usage but the relationship between use and exposure appears more complex at a local scale. Use is likely to be of greater importance. Resistance to ARs in commensal species may also affect exposure in predators. Resistance influences the total amount of AR available to non-targets and should be considered when dealing with rat infestations, as resistance-breakers may present a lower risk to wildlife.
RA22-3

Reflections on the risk of first generation Anticoagulant Rodenticides to Raptors

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In the United States Environmental Protection Agency placed new regulatory restrictions on the use of second generation anticoagulant rodenticides. These changes are expected to result in expanded use of older first generation indandione compounds (FGARs; e.g., diphenacol, chlorophacinone). Recent acute oral and 7-day dietary diphenacol toxicity studies conducted in American kestrels (Falco sparverius) and Eastern screech-owls (Megascops asio) suggest that raptors are considerably more sensitive to FGARs than predicted by data developed with traditional avian wildlife test species (Northern bobwhite, Colinus virginianus and mallards, Anas platyrhynchos). Many studies have shown that the toxicity of FGARs to target rodent pest species is more pronounced in a multi-day exposure scenario. Likewise, some data indicate that the toxicity of FGARs to non-target wildlife is greatly enhanced in a repetitive dietary exposure scenario. Regulatory agencies continue to require and use acute oral toxicity data (i.e., LD50 derived from single or multiple doses administered in a 24-hour period) as a significant component of their ecological risk assessments. While a valuable measure of toxicity, the LD50 can underestimate the toxicity of FGARs that can be more toxic when consumed over several days. Additional information examining the effect of repeated frequency and duration of FGAR exposure would improve risk assessments. Furthermore, sublethal FGAR responses (e.g., bleeding, coagulopathy, histopathological lesions) that may constitute biologically significant adverse effects are considered, but are given less weight in the overall risk assessment. Some of these adverse effects could affect survival of free-ranging birds in ways that would not be apparent in a controlled laboratory setting. Choice of test species, laboratory exposure regimens and toxicity endpoints, as well as better characterization of the probability of exposure in field situations, deserve further attention to more accurately assess the risk that FGARs pose to non-target wildlife.

RA22-4

Investigating the potential risk of secondary rodenticide poisoning to urban owls inhabiting and foraging in urban landscapes of the Lower Mainland, British Columbia, Canada

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Anticoagulant rodenticides are widely used to control pest rodents, but poisoning of non-target wildlife has been linked to these practices, including secondary poisoning of birds of prey, particularly owls. In this study, we investigate whether Barred owls (Strix varia), Great-horned owls (Bubo virginianus) and/or Barn owls (Tyto alba) inhabiting and foraging in predominantly urban landscapes of the Lower Mainland, British Columbia are at risk of consuming rodenticide-laden prey, such as rats and house mice. By conducting a pellet study, we found that urban Barred owls had the highest proportion of rats in their diet, with some individuals’ diet consisting primarily of rats. Urban Great-horned owl pellets were also comprised mainly of rats, but there was a clear shift towards alternative prey base when urbanization within home ranges decreased. Field voles (Microtus townsendii) were the main prey item for Barn owls, regardless of the amount of urbanization within their home range. For all species, consumption of rats and house mice appears to coincide with increased urbanization within home ranges. The shift in the diet of owls living in urbanized areas may potentially lead to an increased risk of secondary rodenticide poisoning. Radio telemetry was deployed to further investigate which landscape features urban Barn owls select as foraging habitat, and whether foraging in proximity to buildings where rodenticide is applied. Urban Barn owls were found to predominantly forage in grass strips along highway interchanges and verges, and untended grass patches within the city. The majority of foraging was done within 100 m of commercial buildings where rodenticide had been applied. These findings will be discussed in conjunction with previous research done on rodenticide residues found in the livers of deceased owls and the current and historic sales of rodenticides in the Lower Mainland, British Columbia.

RA22-5

How the uses of anticoagulant rodenticides influence the distribution of their residues in rodent community?

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In Europe, Anticoagulant rodenticides (AVKs) are regulated as biocides (Directive 98/8/EC) or as plant protection product (Directive 91/414/EE referred as pesticide use hereafter). According to these uses, the active ingredients (a.i.) found in the commercial products and the quantities that are applied in the environment may be very different. Biocide uses of AVKs correspond to a large diversity of a.i. (8 molecules are homologated) which are applied around villages and habitats at relatively small quantities locally. Plant protection is authorized with 3 a.i. only and is commonly realized in eastern France with large amount of bromadiolone poisoned baits (up to 20 kg / ha) over vast areas (e.g., 12,000 ha in 2006) to control Water voles outbreaks. If large mortality events of rodent predators are generally associated to pesticide uses, secondary exposure of wildlife to biocide AVKs is now widely reported. Here, we aim to document the distribution of 8 AVKs in the rodent community according to the uses in eastern France. For each context of use, 2 areas were selected and the localization and intensity of AVKs treatments were characterized as precisely as possible. Then, both target and non-target rodents were trapped in autumn up to 1 km from the place where AVK treatments have been applied. The residues of the 8 AVKs authorized in Europe were measured in the liver and the whole body of 100 specimens selected in each area. Anticoagulant rodenticides were largely distributed in the rodent community of the treated areas whatever the type of uses. In the pesticide area, a high proportion of individuals in both target and non-target species were exposed to bromadiolone (45%) and the high levels of residues in some individuals (> 50,000 ppb in the liver for some Water voles and mice) may explain lethal poisoning of rodent predators. In biocide areas, median liver concentrations of all AVKs were 3.5 and 1.3 ppb in target and non-target species respectively, 23% of the specimens trapped exhibiting detectable residues of AVKs in the liver. This suggests that predators are frequently exposed to low doses of different AVKs but the impact of sublethal exposure of biocides to rodenticides remains under question.

RA22-6

Risk mitigation measures for anticoagulants, used as rodenticides in Sweden

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Anticoagulants used as rodenticides are non-selective, highly toxic substances. Second generation anticoagulants (SGARs) (bromadiolone, difenacoum, brodifacoum, flocoumafen and difethialone) are also persistent with extremely slow elimination from the body, and prone to accumulate in non-target species that consume poisoned rodents (secondary poisoning). They have characteristics which meet the criteria to be classified as potential PBT and potential vPvB substances. Furthermore, monitoring studies in several countries have shown high levels of second generation anticoagulants in predatory mammals, raptors and owls. Nevertheless, SGARs have been included in Annex I to Directive 98/8/EC because of their identified benefits for public health and the lack of established alternatives which are at the same time equally effective and less damaging to the environment.

If SGARs are to be used, extensive risk mitigation measures needs to be applied in order to reduce the risks for primary and secondary exposure for humans, non-target animals and the environment. The Swedish Chemicals Agency finds it appropriate to restrict authorisations of rodenticides containing SGARs to user category “class 1 - professional use with a specific permit”. In combination with other risk mitigation measures, this is considered an appropriate way to reduce the risks yet allowing for effective rodent control.

RA23 - Wastewater effluent discharges: chemical characterisation and understanding potential risks in receiving waters

RA23A-1

The UKWIR Chemicals Investigation Programme

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Recent EU legislation in the field of water and the environment, in particular the Water Framework Directive (WFD), has important implications for the scope and nature of pollution control measures required to protect surface waters. Environmental Quality Standards (EQSs) have been set for substances that hitherto have not been subject to detailed monitoring or control. These standards have, in turn, generated a need for compliance assessment and, where necessary, the development of appropriate control measures. The UK Water Industry has responded to this challenge by collaborating with national environmental regulators to undertake a £25M programme of investigations of contaminants in wastewater, their fate and behaviour in wastewater treatment and their sources within urban sewer catchments. Effort is focused on a range of over sixty contaminants, including priority substances regulated at European level, specific pollutants regulated at national level and a range of substances, including pharmaceuticals, of emerging importance. The project is intended to identify and prioritise substances that are likely to require future action under the Water Framework Directive. It also seeks to establish the sources of different substances and to determine the most effective forms of control, including measures not related to end of pipe treatment. This paper provides an overview of the chemicals investigation programme, describes its key outputs and provides examples of how the results of the programme have been used in order to prioritise proposed future measures to be implemented as part of the WFD. The relative performance of different wastewater treatment processes will be discussed in relation to the achievement of good chemical status for surface waters.
RA23A-3
Occurrence of Pharmaceuticals on a sewage impacted section of a Mediterranean River (Llobregat, NE Spain) and their behaviour under different hydrological climate conditions

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Mediterranean rivers are characterized by high flow variability, strongly influenced by seasonal rainfall. In addition, the river receives effluent discharges of more than 55 000 m³/d, and especially at drought periods, the effluents may represent almost 100% of the total flow of the river. When water scarcity occurs, water flow and dilution capacity of the river is reduced. On the other hand, floods contribute to remobilization of pollutants from sediments. Consequently, the potential environmental risk of pollutants is expected to increase. Besides, due to continuing human pressure from extensive urban, industrial and agricultural activities, contamination levels in Mediterranean rivers are frequently higher than in other European river basins.

1,000 different pharmaceuticals (PhACs) are used in human medicine in the European Union. The main route of PhACs into the aquatic environment is excretion by humans and the direct disposal through domestic wastewater. Despite its previous treatment in WWTPs, depending on the efficiency and chemical properties of the compound are able to pass the treatment plants, as did the presence of isotope peaks (providing some idea of peak identity) for positive and negative ions. Over 40% of positive non-target peaks had sulfur present, attributed mainly to sulfonic acids. In contrast, many homologous series were detected in positive ionisation samples, generally resulting from peptides. A comparison of peak intensities for target and non-target peaks revealed that of the top 20 peak intensities in negative mode, only 4 were target compounds. These were three artificial sweeteners (acesulfam, saccharin and cyclamate) and a pharmaceutical (diclofenac). The remaining non-target peaks are clearly a significant part of the sample, despite the comprehensive target list of environmentally relevant compounds selected for relevance to Swiss conditions and based on experience. Despite not knowing the identity of the non-target peaks, we show here that we can follow target compounds, transformation products and even non-target masses in wastewater effluents using in-house software which is available for public use. The information extracted in the envMass workflow can be used to quantity target and TPs as well as prioritise non-target compounds for identification and track these peaks in future monitoring programs.

RA23A-4
PACs during wastewater treatment and in receiving waters - emerging issues

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Pharmaceutically active compounds (PACs) are emerging contaminants found in surface waters at ppt levels. Thousands of PACs are approved for human/veterinary use, although only a very small percentage of these compounds have been studied in the environment. Some of the most commonly used PACs are sold in hundreds of tonnes/year in the UK alone. PACs enter the environment mainly through insufficiently treated sewage, effluents from manufacturing processes, runoff and sludge (if used as fertiliser or transported to landfill). They are ubiquitous and persistent (due to their continuous introduction into the environment) with synergistic properties. PACs may also be detected in drinking water, which poses a direct risk to humans and raises the issue of contaminated water sources. The necessity of research into PACs is widely acknowledged and the need for action to further improve our understanding of risks posed by PACs is often highlighted. The aim of this presentation is to discuss efficiency of different wastewater treatment processes in the removal of PACs and to raise awareness of two important but under-reported issues relating to the presence and fate of PACs in wastewater and their ecotoxicity. These are: (i) the possibility of under-reporting of the measured concentrations of certain PACs due to lack of routine measurement of these compounds in solids and (ii) the possibility of a significant under or overestimation of toxicity of chiral PACs and incorrect environmental risk assessment due to lack of data on enantiomer-specific fate of these compounds during wastewater treatment and in the environment.

RA23A-5
Assessment of WWTPs efficiency to limit surface water pollution by illicit drugs

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Water contamination resulting from consumption of illicit drugs is a new concern for water management that must be considered, not only because of the social and public health implications, but also in an environmental context, because of the contamination of surface waters by partially treatment efficiency of WasteWater Treatment Plants (WWTPs) discharging contaminated effluents. It is now established that WWTPs influeitts contain illicit compounds at concentration included between several ng/L-1 to several µg/L-1 and leading to surface water pollution by WWTPs effluents. When illicit drugs are mistreated, the existing illicit drug metabolism is impaired, and there is no way to correct these data are mistreated, we decide to study 18 drugs and metabolites and to compare WWTPs removal efficiency as a function of volume capacity and technologies of the treatment trains.

RA23A-6
Are the concentrations of micropollutants responsible for the reduction in wastewater toxicity for gammarids following the application of ozone?

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Micropolitants, which comprise among others pharmaceuticals and personal care products, enter the aquatic environment via secondary treated wastewater and are thus frequently detected in surface waters. To counteract these micropolitants, advanced treatment methods are currently under discussion. In this context the application of ozone is considered as an effective tool. However, its ecotoxicological implications are largely unknown. Therefore, the aquatic toxicity of secondary (“non-ozone”) or ozone treated wastewater was assessed using the feeding rate of the leaf-shredding invertebrate Gammarus fossarum, which is known as a key-species in the ecosystem function of leaf litter breakdown. Two repetitive experiments resulted in significantly higher feeding rates for gammarids exposed to ozone compared to non-ozone treated wastewater. The ecotoxicological implications of these findings are twofold: (i) the oxidation rate of organic micropolitants in wastewater is increased and (ii) the ecotoxicological impact of micropolitants is increased. Therefore, it is important to further study an ozone treated wastewater, with contained hardly any micropolitants (i.e., pharmaceuticals), which was at the same level as wastewater from the same source but additionally treated with ozone. These results suggest the load (concentration) of micropolitants to trigger the effects displayed by the bioassay applied, while alterations in the organic matrix seem to be of minor importance. Hence, the feeding rate of G. fossarum appears to be a well-suited bioassay to indicate alterations in ecotoxicological properties of wastewater due to the application of advanced oxidation processes like ozonation.
.ra21b-1
Do we need expensive advanced treatment of waste waters to prevent feminisation of wild fish?
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The extent and implications of Municipal wastewater effluent (MWWE) of fish in the Canadian environment is currently poorly understood. The objective of this research was to examine the impact of MWWEs on the status of sentinel fish species at various levels of biological organization (cellular to community). Field studies conducted in the fall (2007) and spring (2009) in the Grand River watershed, Ontario, Canada, investigated the cumulative impact of two sewage discharges in an urban environment at reference sites upstream of the municipality of Waterloo, and at an intermediate site located between the two sewage treatment plant sites for Waterloo and Kitchener.

Responses of wild fish [Rainbow Darter (Etheostoma caeruleum) and Greenside Darters (E. blennioides)] were assessed in terms of energy storage (condition factor), and species composition when compared to the fish community upstream or further downstream of the points of effluent discharge. Changes in the species composition and energy utilization (reproduction: in vitro sex steroid production, gonadosomatic indices, and histology) . Both sentinel species collected downstream of both discharges demonstrated greater growth (longer and heavier), however fish were not assimilating additional resources into energy storage (increased condition, liver somatic index).

Exposed male darters had impaired capacity to produce androgens in vitro, lower GSI and altered sperm cell staging. Exposed female fish also had impaired capacity to produce estrogens in vitro. Intersex in male darters collected during the fall downstream of both sewage discharges studied while upstream agricultural and urban reference sites demonstrated low levels of intersex. Pre-spawning darters demonstrated dramatically higher incidence of intersex at both the near-field and far-field exposure sites and increased with additions in gonadosomatic indices and steroids. The fish communities downstream of these two effluents demonstrated differences in abundance, diversity, and species composition compared to the fish community upstream or further downstream of the reductive change. Changes in the composition downstream of the outfalls occurred with larger, more tolerable mobile, more toxic species such as suckers and sunfish becoming more common. The potential exists for a cumulative impact of multiple outfalls of treated wastewater effluents as changes were more pronounced downstream of the second sewage discharge. This research demonstrates the potential cumulative effects of MWWE discharges in Canadian rivers on fish responses at various levels of biological organization.

ra21b-2
Reducing and monitoring toxicity in an industrial effluent, using a regulatory approach
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Between 1997 and 2000 the UK government started to try to regulate complex effluents using Direct Toxicity Assessment (DTA). Sites were selected, effluents screened and then ranked for potential toxicity reduction efforts and monitoring.

In this case study we explore a data set spanning 8 years where we applied these processes for an industrial chemical company, resulting in a collaboration that significantly reduced the final effluent acute toxicity.

Effluents were tested using Tubifex tubifex and Skeletonema costatum bioassays. High toxicity was identified and it was decided that the effluent needed moderating before it could be allowed to be disposed of to river. The toxic samples were analysed and Phenol and formaldehyde were identified as key contaminants. Their contribution to the overall toxicity was calculated using a toxic units approach. Assays were preformed according to the UK EAs Standard Committee of Analysts methods and were carried out every month from 2003 until the present. The most toxic samples taken through the industrial process were analysed for phenol and formaldehyde and found to have high concentrations in the 1000s mg/L range. A new piece of equipment was introduced to scrub these specific chemicals from the effluent before it was discharged to the environment.

Following the introduction of the new plant in 2006, detectable toxicity in the two bioassays dropped significantly and has remained low, apart from one unexplained peak in 2008.

This shows the success of the DTA approach and the potential it has to lead to solutions that work for industry and the regulators in reducing toxic inputs to the environment.

ra21b-3
Evaluating advanced treatment of hospital wastewater
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This study aims to evaluate the importance of hospitals as point sources of pharmaceuticals into the environment and to propose possible measures to minimize the pharmaceutical input. For that purpose, a pilot-scale wastewater treatment membrane bioreactor (MBR) was operated at a Swiss cantonal hospital over one year. Part of the

SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting
MBR permeate was further treated either by powdered activated carbon (PAC), ozone, or photocatalysis (UV/TiO2). Employing robust sampling strategy and quantifying over fifty highly consumed pharmaceuticals by online SPE-LC-MS/MS provides robust and reliable results. Measurements of species-specific resistance determinants as well as multi-resistant Pseudomonas aeruginosa have shown that hospitals release high amounts of antibiotic resistant and multi-resistant bacteria to the environment. Hospitals are also major contributors to the load of contrast media, some antinfectives and anesthetics in the environment. Decentralized hospital wastewater treatment is technically possible and ozonation as well as PAC treatment can be recommended as techniques to reduce pharmaceutical load as well as ecotoxicological effects. For most pharmaceuticals high elimination rates were achieved with both treatments; lowest eliminations were observed for the contrast media diatrizoate and ioxitalamic acid. Elimination efficiencies observed in hospital wastewater treatment were similar to the ones in municipal wastewater treatment. Results will be used to support the legal decision weather or not decentralized hospital wastewater treatment would be an option for Switzerland.

RA23B-6
An examination of the toxic properties of water extracts in the vicinity of an oil sand extraction site
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The industrial extraction of oil sands (OS) in northern Alberta, Canada, has raised concern about the water quality of the nearby Athabasca River. The purpose of this work was to examine the toxic properties of various water extracts on Oncorhynchus mykiss trout hepatocytes. The water samples were fractionated on a reverse-phase C18 cartridge and the levels of light-, medium- and heavy-weight polycyclic aromatic hydrocarbons (PAHs) were determined by fluorescence spectroscopy. Primary cultures of trout hepatocytes were exposed for 48 h at 15°C to increasing concentrations of the C18 fraction corresponding to 0.02, 0.1, 0.5 and 2.5X concentrations from upstream/downstream sites in the Athabasca River, groundwater samples, OS tailings and interceptor well-water samples. Changes in cell membrane permeability, activity of phase I and phase II biotransformation enzymes (cytochrome P4501A and glutathione S-transferase activities), oxidative damage (lipid peroxidation LPO) and genotoxicity (single and double DNA strand breaks) were monitored in post-exposure cells. The water samples produced minor changes in membrane permeability but did increase all the above endpoints at thresholds of between 0.02 and 0.1X the water concentration. The most responsive biomarker was DNA damage but it also offered the least discrimination among sites. LPO was stronger at sites downstream of the industrial operations compared to upstream sites. A decision tree analysis was performed to formulate a set of rules by which to identify the distinctive properties of each type of water sample. The analysis revealed that OS tailings and interceptor waters were characterized by an increased concentration in light PAHs (> 42 µg/L) and this fraction represented more than 85% of the total PAHs. These samples also inhibited GST activity, which could compromise the elimination of genotoxic PAHs present in the system. An analysis of groundwater samples revealed a contamination pattern similar to that for OS tailings. There is a need for more research into specific biomarkers of toxicity from OS tailings compounds such as naphthenic acids, light PAHs among others, which are a characteristic fingerprint of OS extraction activities.
MO 001 Calibration and field deployment of five integrative samplers for the monitoring of indicator and dioxin-like PCB (ECLIPSE project)


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Various integrative samplers, at different stages of development, are now available to estimate time-weighted average (TWA) concentrations of freely dissolved hydrophobic contaminants in aquatic environments. The ECLIPSE project (2009-2011, coord. C Miege, Istria) involves 5 laboratories and aims to calibrate and compare 5 different integrative samplers for the monitoring of indicator and dioxin-like PCB in water: semi-permeable membrane device (SPMD, studied by Istrea), low-density polyethylene strip (LDPE, IFRema), silicone rubber (SRP, Deltas), Chromatherm® (BGM) and monolithic passive sampler (CFIS, LABAQUA).

The first step of the project was the field calibration of these samplers under laboratory conditions. During summer 2009, samplers were exposed under constant agitation and temperature in a stainless steel tank filled with 201 L of PCB contaminated water. A constant PCB concentration of about 1 ng/L was achieved by infusing a large amount of silicone rubber (about 400 kg) into the water phase. Prior to deployment, samplers were spiked with Performance Reference Compounds (PRC) and exposure durations ranged from 1 day to 3 months. After exposure, processing and analysis, samplers were compared in terms of sampling rate, linear uptake phase duration, repeatability and accuracy of calculated TWA concentration.

The second step of the ECLIPSE project was the deployment and comparison of these samplers in real aquatic environments. In summer and autumn 2010, three field campaigns were carried out along the Rhône River and near the lake Le Bourget (France), known to be contaminated by PCB. Using appropriate cages, canisters and holders, studied samplers were exposed simultaneously at an approximate depth of 1 m during 1, 2, 3 and 4 weeks with duplicates and/or triplicates. These field campaigns allowed to compare in-situ ease of use and robustness of the five integrative samplers in addition to repeatability of sampling and TWA concentration estimate.

MO 002 A European interlaboratory collaborative study on the use of passive samplers in monitoring of emerging pollutants

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This study was carried out by the partners in the in-house European project Connective (Coord. J. Balaam, WUR, The Netherlands) which aimed at comparing passive samplers on a European level for the monitoring of emerging pollutants, including pharmaceuticals and personal care products in surface and drinking water.

The result of this study is that the passive sampling technique is a promising tool for the monitoring of emerging pollutants, but more research is needed to confirm this. The next step will be to develop a standard method for the monitoring of emerging pollutants in surface and drinking water.

MO 003 Method for passive sampling of TBT in surface waters using silicone rubber - field application

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Maximum permissible concentrations of tributyltin (TBT) in the aquatic phase are lower than the limits of detection for common analytical methods. Passive sampling can accumulate contaminants from large volumes of water and was suggested as a method for the determination of TBT in surface waters. Analytical aspects of passive sampling using silicone rubber and the determination of parameters to convert sampler uptake into aqueous phase concentrations, i.e. sampler-water partition coefficients as well as diffusion coefficients in sampler material were investigated. Sampler water partition coefficients were higher than expected from octanol water partition coefficients and suffered from the presence of particulate matter. Diffusion coefficients for mono and di-substituted organotin compounds were low, such that diffusion in the sampler is partly controlled by the uptake. This requires that for calculation of aqueous phase concentrations both water boundary layer transport and diffusion in the sampler needs to be taken into account. Several field trials were executed. Samplers were deployed for 6-8 weeks, in harbor areas in the Netherlands and at 6 sites in the UK, on a transect from the tidal limit of the Thames down to the Outer Estuary. This poster describes the method developed as well as results of the field and evaluates the applicability of silicone rubber as a suitable passive sampler for butyltin compounds.

MO 004 Comparison of uptake rates of pharmaceuticals and organophosphate flame retardants in a range of passive samplers

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Passive samplers have been widely used to compare contaminants in different studies. In this range of passive samplers (Chemcatcher (polar), Chemcatcher (non-polar), PCOIS, SPMD and PDMS (silicon rubber)) were assessed in a laboratory study. The samplers were deployed in a tank with a continuous flow of water from a header tank, which was set at a rate to allow complete replacement of the water in 30 minutes. Into the header tank, a known concentration of chemical was dosed. Compounds investigated were pharmaceuticals and Organophosphate flame retardants.

The purpose of this tank test is to determine suitability of each of the four samplers in the analysis of these compounds, and to establish sampling rates for the compounds of interest.

The water replenishment meant that we could be confident that any removal of the contaminant by samplers was not sufficient to significantly reduce the concentration of that contaminant in the water phase (meaning that the concentration should be assumed to be constant). Samplers were removed from the tank weekly and the study was terminated after four weeks exposure. Samplers were then extracted and the extracts analysed for the spiked compounds. Relative uptake rates of various compounds to different samplers were established.

MO 006 Simultaneous quantitative analysis of pesticides including Phenoxy-Acids in surface water using UPLC-MS/MS with direct injection

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LC/MS/MS is widely used, in combination with solid phase extraction techniques, to achieve the very low detection levels (low ppt range) needed for the monitoring of pesticides and other pollutants like pharmaceutical drugs in surface and drinking water. Various approaches are possible, depending on the performances on the MS instrument, on the needed sensitivity and on the nature of the sample (drinking or surface water). SPE is usually done off-line, starting from a large volume of water (up to 500 ml to 1 l), with associated drawbacks (long protocols, transportation of the samples, cost). Preconcentration can also be done automatically on-line, with different draw back since the analytes are concentrated from different water. The evolution of the methodology for surface water.

The LC-MS/MS method that we present has been developed for the quantitative analysis of pesticides including phenoxy-acids. The chromatographic separation is done using a Waters Xevo TQ-S tandem-quadrupole mass spectrometer. The MS detector is a Waters Xevo TQ-S tandem-quadrupole mass spectrometer. Such trials are essential to further validate this sampling principle and to increase the confidence of the technological approach for end users. An inter-laboratory study on the use of passive samplers for the monitoring of emerging pollutants was organised in 2011 by the NORMAN association (Network of reference laboratories for monitoring emerging environmental pollutants; www.norman-network.net) together with the European DG Joint Research Centre and the Common Implementation Strategy of the WFD. Thirty academic, commercial and regulatory laboratories participated in the passive sampler comparison exercise and each was allowed to select their own sampler design. All the different devices were exposed at a single sampling site to treated waste water from a large municipal treatment plant. In addition, for each target analyte class the organisers deployed in parallel, multiple samplers of a single type which were subsequently distributed to the participants for analysis. This allowed an evaluation of the contribution of the different analytical laboratory procedures to the data variability. The results obtained allow an evaluation of the potential of different passive sampling methods for monitoring selected emerging organic pollutants (pharmaceuticals, polar pesticides, steroid hormones, fluorinated surfactants, triclosan, bisphenol A and brominated flame retardants). The exercise was a great learning experience for organisers and participants. The results will be used to inform EU Member States about the potential application of passive sampling methods for monitoring these compounds within the framework of the WFD.
preparation, the UPLC column lifetime was several thousand injections. This method brings a significant gain in time (acidic and basic compounds in a single injection), and in cost (sample preparation is limited to filtration). Possible developments on this method is the inclusion of other molecules, including PPCP (Pharmaceutical and Personal Care Products).

MO 007
Monitoring trials for detection of ionic herbicide residues in water using passive samplers

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Passive samplers for routine monitoring of pesticide residues in irrigation channels and rivers have already been developed for a number of hydrophobic compounds. However, some polar, hydrophilic ionic herbicides such as glyphosate and amitrole are either not retained in such samplers or are difficult to dislodge from membranes specifically designed to capture polar compounds. Development of new passive sampling devices for such herbicides required first the development of a suitable analytical method for determination of their residual amounts in environmental samples. An elute chemical detector fitted to a HPLC system detected with accuracy and sensitivity these other common herbicides found in agricultural waters (1). Secondly, SDB-RPS Empore® disk membranes were found to perform best for accumulating amitrole, and were chosen for calibrating a passive sampling device containing these membranes under flow-through laboratory conditions. Whilst SDB-XC Empore® disk membranes could be used to collect fluorescent glyphosate from spiked water samples filtered through them, this membrane was unable to accumulate this herbicide in a flow-through system. Instead, glyphosate accumulated in a passive sampler device consisting of Amberlite® IRA67 resin pre-washed with 1M NaCl, dried and then packed in nylon mesh bags (240 micron) that were subsequently tested under the same flow-through laboratory conditions. Both herbicides could be extracted from their respective samplers by the same extraction method using 10 mM NaOH, which facilitated the processing and analysis of the herbicides taken up by the passive samplers. A field trial to test the performance of both types of sampling devices when deployed in agricultural irrigation channels was carried out. Results from the field trials are still under way, and will be presented to show whether the mean time-integrated pesticide concentrations taken up by the passive samplers compare with the cumulative mean water concentrations calculated from daily extractions using the Empore disk membranes.

MO 008
In-situ validation of 3 PRCs and calibration of 14 pharmaceuticals and 20 endocrine disruptors on the polar C18 Chemcatcher

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A wide variety of environmental compounds of concern, e.g. pharmaceuticals or illicit drugs, are acids or bases that may be predominantly present as charged species in drinking water sources. These charged micro pollutants happen to exist in the environment in large numbers due to anthropogenic activities. Many of these compounds have a high affinity towards water and are often difficult to dislodge from membranes specifically designed to capture neutral compounds. Therefore, sorption materials allowing coulomb interaction are often used to enable sampling of these compounds. Detailed knowledge on their sorption behaviour, however, is sparse, especially concerning passive sampling in environmental monitoring. The exact influence of both the charged and the neutral moiety on the sorption behaviour is not yet well investigated. The presence of charged organic ions (e.g. Ca2+, Cl−), that are commonly present in water, on the sorption affinity is just as little understood.

For this research sorption coefficients in different water matrices for various charged compounds, such as pharmaceuticals and chemical liquids, were derived from measured retention times on columns filled with ion exchangers and SDB as inert support material. The results show that polar interaction of charged compounds with the sorption material is an important factor regarding sorption affinity. The more pronounced the apolar moiety is, the higher the sorption coefficients. Equally important is the influence of various inorganic ions in the water phase. This study shows that for e.g. metformin changing from Ca2+ to Na+ the sorption coefficients on a cation exchanger rise by one order of magnitude.

These results help to evaluate if the use of passive samplers for a compound is useful under certain conditions. It becomes clear that sampling in e.g. Ca2+ rich water is more challenging than in Na+ containing water and that small organic ions with a lack of apolar moieties are difficult to concentrate on a passive sampling materials so far.

MO 009
Development of novel monitoring, analytical chemistry and modelling methods for improving the ecological risk assessment of radioactive caesium in the aquatic environment in East Japan

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Polar Organic Chemical Integrative Samplers (POCIS) have been originally developed for sampling polar compounds from the aquatic environment. As a passive sampling method, POCIS consist of an adsorbent material which is an important factor regarding sorption affinity. The more pronounced the apolar moiety is, the higher the sorption coefficients. Equally important is the influence of various inorganic salts in the water phase. This study shows that for e.g. metformin changing from Ca2+ to Na+ the sorption coefficients on a cation exchanger rise by one order of magnitude.

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MO 010
Monitoring trials for detection of ionic herbicide residues in water using passive samplers

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MO 011
Calibration data for Polar organic chemical integrative samplers (POCIS)

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Polar Organic Chemical Integrative Samplers (POCIS) have been originally developed for sampling polar compounds from the aquatic phase. POCIS consist of an adsorbent material which is an important factor regarding sorption affinity. The more pronounced the apolar moiety is, the higher the sorption coefficients. Equally important is the influence of various inorganic salts in the water phase. This study shows that for e.g. metformin changing from Ca2+ to Na+ the sorption coefficients on a cation exchanger rise by one order of magnitude.

These results help to evaluate if the use of passive samplers for a compound is useful under certain conditions. It becomes clear that sampling in e.g. Ca2+ rich water is more challenging than in Na+ containing water and that small organic ions with a lack of apolar moieties are difficult to concentrate on a passive sampling materials so far.

MO 012
In-situ validation of 3 PRCs and calibration of 14 pharmaceuticals and 20 endocrine disruptors on the polar C18 Chemcatcher

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In response to the growth of organic pollutants identified in surface water many multi-residue analytical methods have been developed to quantify multi-families of emerging pollutants in water. Many strategies include enrichment steps for water samplings due to very low levels of pollution [1]. Recently, sampling systems more realistic of
environmental exposure have been designed to get time weighted average (TWA) concentrations of those xenobiotics. Those passive samplers enable further investigation for toxicological effects on the environment or populations of such mixture and concentrations.

The polar C18 Chemcatcher has been evaluated for the monitoring of multi-families of Endocrine Disruptors and Pharmaceuticals. First C18 Chemcatcher with PES diffusion membrane was calibrated for POCIS approach (Permeation Oriented Chemical Integrative Samplers). Scientists have been exposed for 28 days in a 50L flow through microcosm for the adsorption study and spiked samples with tap water for the desorption experiment. Finally samples were exposed for 3, 7, and 14 days in surface water in two rivers near Lyon.

All these calibrated molecules showed good correlation to first order accumulation with half time of equilibrium above 14 days for most of those molecules. Good linear relationships were obtained (R² from 0.90 to 0.99) for 7 to 21 days on the C18 Chemcatcher. Sampling rates were calculated between 0.005 and 0.16 L·d⁻¹. Most samples showed accumulation and desorption consistent with first order kinetics with similar half time of equilibrium and thus verifying all criteria for their use as PRC. Exposure campaign allows to validate PRCs comparing TWA concentrations obtained from passive samplers to average concentrations detected in grab sampling analyzed by online SPE- LC-MS/MS method.

References

MO 013

Comparison of active pesticide analysis via traditional surface water sampling and Chemcatcher® passive samplers

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Pesticide monitoring in European surface waters is regulated by the Water Framework Directive (WFD) establishing environmental quality standards (EQS) for the good chemical status of water bodies. EQS monitoring is based on analyses of pesticide in water samples. WFD requires at least monthly sampling for assessment of maximum annual average concentrations. Due to the high temporal variation of pesticide use and leaching and discharge conditions in running waters, such robust monitoring approach may fail to detect pesticides, especially peak concentrations. We compared traditional water sampling results to pesticide concentrations detected with Chemcatcher® passive samplers in a large peatland river in Kyrojoki and its small tributary Lehmajoji. The Chemcatcher® were deployed in four separate trials on both sites for two weeks time period during 21 Jan - 30 Aug. The traditional water samples were analysed twice a month in Lehmajoji and monthly in Kyrojoki.

The number of compounds found in Chemcatcher® was 52, while in water samples 27 pesticides were detected but only 15 of them were quantified. High concentrations of some compounds were found twice in Chemcatcher® and three times in water samples. The preliminary results clearly indicate that measurement of pesticides from water samples is prone to failures to detect their actual presence in water bodies. Passive sampling with Chemcatcher® should also be compared simultaneously with other methods which have commonly been used earlier in monitoring organic pollutants, like natural biota, sediments and bioaccumulation using mussels.
Impact of biofouling on DGT measurements in water

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The bioavailability of PAHs in the seawater by using SPMDs were carried out in the Potiguar basin, located at Rio Grande do Norte State, Brazil. The SPMDs were deployed in the three different months of the year at five sampling points. Three sampling points were located near an ocean outfall which discharges produced water and two at 12 Km distant from the outfall, as a reference area. It was analyzed the EPA’s 16 priority pollutant PAHs and the respective homologue alkylated compounds. Near the outfall concentrations ranged from 25 ng L\(^{-1}\) to 223 ng L\(^{-1}\) with the presence of alkylated compounds from 2 to 4 rings and presenting PAHs distribution with weathering characteristics. In the control area the total PAHs concentrations were quite similar to the blank sample, ranging from 0.8 ng L\(^{-1}\) to 4.8 ng L\(^{-1}\). PAHs concentration found in seawater near the outfall was within the concentration expected by the dilution model of the effluent. To sum up, based on this study, the SPMD technique has shown considerable promise in studies in tropical and eutrophic waters.

Use of the semipermeable membrane devices (SPMD) as integrative tool for monitoring polycyclic aromatic hydrocarbons in tropical seaway


Petropolis, Rio de Janeiro, Brazil

Pontificia Universidade Católica (PUC-Rio), Rio de Janeiro, Brazil

To assess PAHs in the seawater by using SPMDs were carried out in the Potiguar basin, located at Rio Grande do Norte State, Brazil. The SPMDs were deployed in the three different months of the year at five sampling points. Three sampling points were located near an ocean outfall which discharges produced water and two at 12 Km distant from the outfall, as a reference area. It was analyzed the EPA’s 16 priority pollutant PAHs and the respective homologue alkylated compounds. Near the outfall concentrations ranged from 25 ng L\(^{-1}\) to 223 ng L\(^{-1}\) with the presence of alkylated compounds from 2 to 4 rings and presenting PAHs distribution with weathering characteristics. In the control area the total PAHs concentrations were quite similar to the blank sample, ranging from 0.8 ng L\(^{-1}\) to 4.8 ng L\(^{-1}\). PAHs concentration found in seawater near the outfall was within the concentration expected by the dilution model of the effluent. To sum up, based on this study, the SPMD technique has shown considerable promise in studies in tropical and eutrophic waters.

MO 022

Development and application of a passive sampling technique for determining biomagnification factors and elimination half-lives in fish following dietary exposure

R.G. Manning1, J. Guo1, D.J. Letinski1, J.D. Butler1, M.J. Connolly1, T.F. Parkerton1, M.A. Lamps1

ExxonMobil Intellectual Property and Research, Annandale, United States of America

The objective of this study was to develop and evaluate a passive sampling technique for determining biomagnification factors (BMF) and elimination half-lives (t\(_{1/2}\)) of contaminants in fish following dietary exposure. BLMs were deployed near a fish farm in New Jersey, United States of America

ExxonMobil Petroleum & Chemical, Machesen, Belgium

Recent revisions to the OECD 305 test protocol have led to the introduction of a dietary exposure test in which the bioaccumulation potential of a substance is characterized in seawater using polycyclic aromatic hydrocarbons (PAHs) as a proxy for the accumulation of hydrophobic contaminants. The BLM technique is based on the basic idea of mimicking the uptake of lipophilic contaminants by the fish in their natural environment. BLMs deployed in the Potiguar basin, located at Rio Grande do Norte State, Brazil. The BLMs were deployed in the three different months of the year at five sampling points. Three sampling points were located near an ocean outfall which discharges produced water and two at 12 Km distant from the outfall, as a reference area. It was analyzed the EPA’s 16 priority pollutant PAHs and the respective homologue alkylated compounds. Near the outfall concentrations ranged from 25 ng L\(^{-1}\) to 223 ng L\(^{-1}\) with the presence of alkylated compounds from 2 to 4 rings and presenting PAHs distribution with weathering characteristics. In the control area the total PAHs concentrations were quite similar to the blank sample, ranging from 0.8 ng L\(^{-1}\) to 4.8 ng L\(^{-1}\). PAHs concentration found in seawater near the outfall was within the concentration expected by the dilution model of the effluent. To sum up, based on this study, the SPMD technique has shown considerable promise in studies in tropical and eutrophic waters.

MO 021

Use of the semipermeable membrane devices (SPMD) as integrative tool for monitoring polycyclic aromatic hydrocarbons in tropical seawater

ExxonMobil Intellectual Property and Research, Annandale, United States of America


Petropolis, Rio de Janeiro, Brazil

Pontificia Universidade Católica (PUC-Rio), Rio de Janeiro, Brazil

To assess PAHs in the seawater by using SPMDs were carried out in the Potiguar basin, located at Rio Grande do Norte State, Brazil. The SPMDs were deployed in the three different months of the year at five sampling points. Three sampling points were located near an ocean outfall which discharges produced water and two at 12 Km distant from the outfall, as a reference area. It was analyzed the EPA’s 16 priority pollutant PAHs and the respective homologue alkylated compounds. Near the outfall concentrations ranged from 25 ng L\(^{-1}\) to 223 ng L\(^{-1}\) with the presence of alkylated compounds from 2 to 4 rings and presenting PAHs distribution with weathering characteristics. In the control area the total PAHs concentrations were quite similar to the blank sample, ranging from 0.8 ng L\(^{-1}\) to 4.8 ng L\(^{-1}\). PAHs concentration found in seawater near the outfall was within the concentration expected by the dilution model of the effluent. To sum up, based on this study, the SPMD technique has shown considerable promise in studies in tropical and eutrophic waters.

MO 020

Evaluation of different passive samplers to predict uptake of polycyclic aromatic hydrocarbons by crop plants

J.G. Collings

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Polycyclic aromatic hydrocarbons (PAHs) belong to a class of ubiquitous organic pollutants, produced during the incomplete combustion or pyrolysis of organic materials from primary anthropogenic sources such as fossil fuels and agricultural waste. The fate of PAHs in the nature is of great concern to human health as these contaminants are widely distributed in the environment and are known to be persistent, mutagenic and carcinogenic. In the past decades, passive sampler devices (PSDs) have been developed to concentrate hydrophobic organic compounds (HOCs) from environmental matrices and to mimic bioconcentration. Previous research has indicated that tetrone embedded cellulose acetate membrane (TECAM) and polycarbonate embedded cellulose acetate membrane (PECAM), types of lipid containing membranes as well as sample made of polydimethylsiloxane (PDMS) have potential to accumulate certain polycyclic aromatic hydrocarbons (PAHs) from water and soil and to estimate the bioavailability of these pollutants to living organisms. The present study compares the ability of this suite of passive samplers to mimic uptake of 15 PAH prioritised by the European Scientific Committee on Food (ESC) by crop plants grown in a hydroponic nutrient solution.

MO 019

Vertical fluxes of Polycyclic Aromatic Hydrocarbons in the Pelegrino Field (Southeastern Brazilian Shelf): preliminary results

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Pelegrino Field is a region located at 23°20’S - 41°12’W on Southeastern Brazilian Shelf that recently has being explored for petroleum resources. Therefore, the adjacent marine environment may be impacted by the introduction of material from drilling activities. Polycyclic aromatic hydrocarbons (PAHs) are an important proxy for the identification of this impact because they are present in petroleum and its products, indicating introduction of these materials in the marine environment. Sediment traps are a passive sampling tool used to monitor the impact caused by drilling activities. The aim of this study is to evaluate the amounts and fluxes of PAHs on Pelegrino field. Setting suspended matter (SSM) were sampled using two sediment traps (S1 - 23°18’S, 41°13’W; and S3 - 23°18’S, 41°12’W) equipped with 20 cups filled with mercury chloride (HgCl2) to prevent organic matter bacterial degradation. The sediment trap area was 0.650 m² and sampling interval was three days. PAHs concentrations were determined by gas chromatography coupled to mass spectrometer detector (GC/MS). Overall, PAHs concentrations suggest a low level of contamination, since levels were lower than 250 ng g\(^{-1}\). PAHs amounts show no difference between S1 and S3. Total PAHs (parental and alkylated PAHs) ranged from 12.2 to 687 ng g\(^{-1}\), with similar average for both sediment traps S1 and S3. There is a large difference between amounts and proportions of low molecular weight (LMW) and high molecular weight (HMW) PAHs. S1 presented on average 48.9% of LMW and 51.1% of HMW, while S3 showed 42.2% of LMW and 57.8% of HMW. It suggests a mixture of PAHs derived from both petrogenic and pyrolytic sources on the SSM, which may result from both drilling and settling activities in the area. SSM vertical flux shows a great difference between S1 and S3, with negative fluxes of 600 ng m\(^{-2}\) d\(^{-1}\) and 381 ng m\(^{-2}\) d\(^{-1}\). This was reflected on total PAHs fluxes. S1 ranged from 10.4 to 317 ng m\(^{-2}\) d\(^{-1}\), while S3 ranged from 43.2 to 240 ng m\(^{-2}\) d\(^{-1}\). Although PAHs levels were similar between S1 and S3, vertical fluxes showed that S3 area exports more PAHs through the water column suggesting that S3 area is being more impacted by drilling activities than S1.
Study of partitioning between lipid and passive sampling materials for equilibrium sampling
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TNO, Utrecht, Netherlands

Sampling using one or more methods phase semi permeable membrane devices (SPMDs) as well as single phase polymer samplers (e.g. polydimethylsiloxane (PDMS), low density polyethylene (LDPE)) are widely used for monitoring of hydrophobic contaminants in the aqueous environment. Application of such passive samplers can be extended to monitoring of hydrophobic contaminants in fish tissue. Equilibrium concentration in PDMS sheets immersed in fish tissue can be easily converted to a concentration on lipid and passive mask (Klps) and reported in literature. Klps can be calculated as the ratio of contaminant concentration in each phase at equilibrium. In the present work partitioning of major groups of hydrophobic contaminants as PCP, PAHs, BDEs and various pesticides between these polymer materials (e.g. PDMS, LDPE) and various pesticides (e.g. octanol, fish, seal oil and a model lipid, troeol) is studied. The influence of temperature on the Klps is investigated. Equilibrium is confirmed by using performance reference compounds (PRCs) with properties equal to the properties of target compounds. Target compounds and PRCs are dosed to different media and an equal distribution of both compounds after equilibration demonstrates that equilibrium is achieved. Additionally different passive sampling materials can be characterized by multiple reaction monitoring (MRM) and analyzing the lipid patterns. The Klps values will contribute to implementation of monitoring in biota through passive sampling. Additionally when combined with existing water-LDPE partition coefficients, the obtained troeol-LDPE partition coefficients also to estimate water-SMID partition coefficients for comparison with values presently applied in water passive sampling.

Implementing WFD biota standards - a possible role for passive samplers?
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Environment Agency, Westminster, Ireland
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Environmental Quality Standards (EQS) define tolerable upper limits for concentrations of chemicals in the environment. For some substances, there is now the option of monitoring compliance in the body tissues of aquatic biota, or sediments. This may offer a more reliable and cost-effective measure of potential environmental risk than measurements in the water column for substances that bio-accumulate strongly and have very low aqueous EQSs.

Under the EU EQS Daughter Directive (EQSD), biota standards have been set for:

- mercury;
- hexachlorobenzene (HCB); and
- hexachlorobutadiene (HCBD).

The EU EQS identifies a requirement for biota monitoring. The use of biota for assessing compliance and trends presents a number of challenges, e.g. choice of appropriate species, availability of species at different sites, and the required monitoring of large numbers of fish or invertebrates to collect the required data. We are not yet at a stage where we can implement biota standards with confidence.

To do so, one needs to be exploring alternative ways for assessing biota standards and trend monitoring under the WFD. In this study, we have measured with the help of semipermeable membrane devices, silicone strips and low density polyethylene membranes dissolved phase concentrations of a number of lipophilic organic contaminants in biota, including polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDDs and PCDFs) and polybrominated diphenyl ethers (PBDEs). Reconciliation between passive sampling measurement and EQS is needed. Derivation of EQS values for the truly dissolved phase is a long-term option. A shorter-term initiative may be to estimate river-specific suspended particle matter-water partitioning coefficients. These may be based on the measured water:sediment partition coefficient of the dissolved phase with passive samples combined with techniques such as continuous flow centrifugation and in situ integrative SPMD samplers. In this study, we have measured the importance of the use of semipermeable membrane devices, silicone strips and low density polyethylene membranes in monitoring of hydrophobic contaminants in Norwegian rivers.

Measuring contaminant partitioning in Norwegian rivers
I.J. Allan, S.B. Rannekleiv, C. Harman

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Chemical monitoring under legislative structures such as the European Water Framework Directive (WFD) heavily relies on the application of environmental quality standards (EQS). Under the WFD, EQS values for hydrophobic organic priority substances have been set for the "whole water". Conventional sampling-analytical methodologies fail to meet target performance sampling criteria for WFD method selection. Passive sampling devices are able to provide improved limits of detection (when compared with bottle sampling) and time-integrated measurements. However, concentrations measured with passive samplers are for the truly dissolved fraction and do not include those bound to particle or dissolved organic matter (i.e. the "whole water"). Reconciliation between passive sampling measurement and EQS is needed. Derivation of EQS values for the truly dissolved phase is a long-term option. A shorter-term initiative may be to estimate sample-specific suspended particle matter-water partitioning coefficients. These may be based on the measured water:sediment partition coefficient of the dissolved phase with passive samples combined with techniques such as continuous flow centrifugation and in situ integrative SPMD samplers. In this study, we have measured the importance of the use of semipermeable membrane devices, silicone strips and low density polyethylene membranes in monitoring of hydrophobic contaminants in Norwegian rivers.

Development of passive surrogate addditive devices for remote water sampling
J. Hong, T. Onde

Waters, Goyancourt, France

The attempt of ensuring safety following an oil spill, a rapid screening method is required to analyze food for compounds of concern. Of the many compounds found in oil, PAHs are of specific concern because they are polycyclic aromatic hydrocarbons (PAHs). These compounds are known to be carcinogenic and the US Environmental Protection Agency has defined these compounds as priority pollutants.

The application of ambient desorption techniques for sample introduction into mass spectrometers is an emerging technology that has applicability in many areas of contaminants analysis. The atmospheric-pressure solids analysis probe (ASAP) is a unique mass spectrometry technique for direct analysis of volatile, semi-volatile, solid and liquid samples. In ASAP, samples are introduced to the mass spectrometer on a glass capillary and vaporized with heated nitrogen desolvation gas. Ionization is achieved using ambient desorption techniques.

Development of ambient desorption techniques for rapid mass spectrometric analysis of contaminants
J. Hong, T. Onde

Waters, Goyancourt, France

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Ambient thermal desorption ionization for rapid mass spectrometric analysis of contaminants
J. Hong, T. Onde

Waters, Goyancourt, France

To ensure the safety of consumers following an oil spill, a rapid screening method is required to analyze food for compounds of concern. Of the many compounds found in oil, PAHs are of specific concern because they are polycyclic aromatic hydrocarbons (PAHs). These compounds are known to be carcinogenic and the US Environmental Protection Agency has defined these compounds as priority pollutants. To ensure the safety of consumers following an oil spill, a rapid screening method is required to analyze food for compounds of concern. Of the many compounds found in oil, PAHs are of specific concern because they are polycyclic aromatic hydrocarbons (PAHs). These compounds are known to be carcinogenic and the US Environmental Protection Agency has defined these compounds as priority pollutants. To ensure the safety of consumers following an oil spill, a rapid screening method is required to analyze food for compounds of concern. Of the many compounds found in oil, PAHs are of specific concern because they are polycyclic aromatic hydrocarbons (PAHs). These compounds are known to be carcinogenic and the US Environmental Protection Agency has defined these compounds as priority pollutants.
Ultra low level determination of bisphenol A, 17-β estradiol and poly aromatic hydrocarbons in river water using fully automated column-stitching HPLC

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柱状ストッチング装置の一つであるSPE装置の用途、特に環境試料分析への応用について考察した。SPE装置の選択、前処理の選択、前処理後の溶出の選択等、環境試料分析への応用を以下の通り考察した。

HPLC analysis of polycyclic aromatic hydrocarbons in tobacco smoke using a quartz column

A. Brogat, E. Baures, O. Thomas, B. Roig

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The suitability of coconut charcoal as a sorbent for the determination of N-nitrosamines in water has been investigated. The results showed that coconut charcoal is an effective sorbent for N-nitrosamines, with high sorption efficiency and selectivity. The use of coconut charcoal as a sorbent can provide a simple and cost-effective method for the determination of N-nitrosamines in water samples.

MO 028
Development of a communicating portable analytical system of organic micropollutants in water based on UV spectrometry-fluorimetry detection after multiple solid phases selective preconcentration

M.A. Brogat, E. Baures, O. Thomas, B. Roig

EHESS/CERES, Rennes, France

11Shimadzu Corporation, Kyoto, Japan


2CURETEX CORPORATION, Fukui, Japan


MO 029

Ultra low level determination of bisphenol A, 17-β estradiol and poly aromatic hydrocarbons in river water using fully automated column-stitching HPLC

Y. Watabe1, T. Hayaokawa1, T. Tangawa2, T. Kubo3, K. Hosoya

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Kyoto prefectural university, Kyoto, Japan

MO 030
Development and calibration of a passive sampler for N-nitrosodimethylamine (NDMA) in water

S.L. Kaserzon1, K. Kennedy1, D.W. Hawker1, N. Holling1, B.L. Escher1, K. Boop1, J.M. Mueller1

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MO 031

Development and calibration of a passive sampler for N-nitrosodimethylamine (NDMA) in water

S.L. Kaserzon1, K. Kennedy1, D.W. Hawker1, N. Holling1, B.L. Escher1, K. Boop1, J.M. Mueller1

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N-Nitrosamines as N-nitrosodimethylamine (NDMA) are organic compounds of contemporary interest in environmental waters, including groundwater, wastewater and potable water, due to their carcinogenicity in laboratory animal studies and probable human carcinogenicity. Heightened awareness of their properties and prevalence has led to increased scrutiny of water with Maximum Contaminant Level (MCL) goals ranging from 2 ng L-1 in California to 10 ng L-1 respectively in Canada and Australia and quantification limits down to low ng L-1 levels.

USEPA Method 521 [1] for the analysis of N-nitrosamines in water is a coconut charcoal-based solid phase extraction method. This work investigated the use of the charcoal specified in this method as a passive sampler sorbent for NDMA and stipulates its use for other nitrosamines.

The suitability of coconut charcoal as a sorbent for the determination of NDMA has been previously investigated. However, this involved simple batch experiments. To employ it in a passive sampler, calibration data such as sampling rates (Rs L.day-1) and sampler-water sorption coefficients (KSW) applicable to environmental conditions must be available for targeting and controlling detection and quantification efficiencies independent of ambient concentrations. The aim of this study then was to develop and calibrate a passive sampler for NDMA using coconut charcoal as a sorbent phase.

MO 032

‘Wa-shi’ (Japanese paper) fabrics as adsorbents

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1Kyoritsu Prefectural University, Kyoto, Japan

MO 033

近日来，含二塩基アミン（N-nitrosamines）の環境試料分析への応用が注目されている。本研究では、N-nitrosodimethylamine (NDMA) の定量法であるUSEPA Method 521 を用いたカクシン活性炭セパレータを用いた新しいビームロースキナーの開発を試みた。
Passive dosing as a tool to recreate the environmental mixture composition of HOCs in an aquatic toxicity test

MO 034
P. Babica,1 The University of Queensland, Coopers plains, Australia
Field evaluation of chemical probes to determine the fate of persistent organic pollutants in soil under Grant Agreement No. 229603 and co-financed by the South Moravian Region.

Polychlorinated biphenyls (PCBs) and polychlorinated naphthalenes (PCNs) by means using passive samplers have several drawbacks, such as high cost or power need. Consequently, alternative methods, such as passive samplers, are being developed, as semi-quantitative measures of the distribution of POP in the environment. POP accumulation in low temperature environments such as the polar regions and mountains is described as cold trapping. In order of the contaminants physico-chemical properties, especially to introduce this approach to drinking water treatment industry for control and management of cyanotoxins.

MO 035
P. Babica1, P. Mayer2, H.C.H. Lützhøft1, P.S. Mikkelsen1

The general aim of this study was to explore the potential of passive dosing for testing the toxicity of a PAH mixture that recreates the mixture composition found in seawater from a coastal area of Spain, the Bay of Algeciras. First, solvent spiking and passive dosing were compared for their suitability to detect the acute toxicity to A. franciscana nauplii of several PAHs at their respective solubility limits. Second, passive dosing was applied to recreate the seawater mixture composition of PAHs from a Spanish coastal area, and to test the toxicity of the biotoxin mixtures at different levels. HPLC analysis was used to determine the reproducibility of the dissolved exposures concentrations for the individual PAHs and mixtures. These studies show that passive dosing has some important benefits in comparison with solvent spiking for testing hydrophobic organic compounds (HOCs) in aquatic media. These include maintaining constant exposure concentrations, therefore higher reproducibility and a relative increase in toxicity. Passive dosing is also able to faithfully reproduce real mixtures of HOCs, such as PAHs, in appropriate toxicity tests, reproducing both the levels and proportions of the different compounds. This provides a useful approach for studying the toxicity of environmental mixtures of HOCs, with a view to investigating their toxicity but also for increasing safety factors than those provided by traditional techniques to monitor cyanobacteria and microorganisms in two different water reservoirs and adjacent drinking water treatment plants in the Czech Republic. During the sampling period Jul-Nov 2011, passive samples were biweekly deployed/replaced and grab samples collected from open reservoirs and from different stages of water treatment process (raw water, flocculation, clarification, filtration, final treated water). Phytoplankton species composition and quantities were determined microscopically as well as by submersible fluorimeters. Microcystin concentrations were determined in both grab samples and exposed passive samples by HPLC-DAD and/or immunochromatographically (ELISA). The poster will compare data obtained from both sampling approaches (passive/gear sampling) as well as discuss and demonstrate potential and limitations of passive sampling techniques for monitoring cyanotoxins in drinking water, drinking water quality control, evaluation of efficiency of cyanotoxin removal during drinking water treatment processes, a human health risk assessment. This study should facilitate future applications of passive sampling techniques in water quality monitoring practices.

MO 037
M. Laxander, T. Schiedek, C. Schueth

We also demonstrate how to overcome this limitation with a novel dosing technique where the polychlorinated dibenzo-p-dioxins are desorbed from a polymer. This study shows that passive dosing has some important benefits in comparison with solvent spiking for testing hydrophobic organic compounds (HOCs) in aquatic media. These include maintaining constant exposure concentrations, therefore higher reproducibility and a relative increase in toxicity. Passive dosing is also able to faithfully reproduce real mixtures of HOCs, such as PAHs, in appropriate toxicity tests, reproducing both the levels and proportions of the different compounds. This provides a useful approach for studying the toxicity of environmental mixtures of HOCs, with a view to investigating their toxicity but also for increasing safety factors than those provided by traditional techniques to monitor cyanobacteria and microorganisms in two different water reservoirs and adjacent drinking water treatment plants in the Czech Republic. During the sampling period Jul-Nov 2011, passive samples were biweekly deployed/replaced and grab samples collected from open reservoirs and from different stages of water treatment process (raw water, flocculation, clarification, filtration, final treated water). Phytoplankton species composition and quantities were determined microscopically as well as by submersible fluorimeters. Microcystin concentrations were determined in both grab samples and exposed passive samples by HPLC-DAD and/or immunochromatographically (ELISA). The poster will compare data obtained from both sampling approaches (passive/gear sampling) as well as discuss and demonstrate potential and limitations of passive sampling techniques for monitoring cyanotoxins in drinking water, drinking water quality control, evaluation of efficiency of cyanotoxin removal during drinking water treatment processes, a human health risk assessment. This study should facilitate future applications of passive sampling techniques in water quality monitoring practices.

MO 038
L. Vierow, M. Stahl, M. Schlüschner, J.L. Domingo

High-volume active samples have been conventionally used for the environmental monitoring of persistent organic pollutants (POPs) in air. However, these systems have severe limitations, high cost or power inefficiencies. Such passive samplers, being developed, are semi-quantitative measures complementing active systems. Due to the low cost and easy handling, polyurethane foam (PUF) disks are especially attractive. PUFs seem to be a useful tool to compare the state of pollution in specific areas, as well as for seasonal and spatial distributions of local POPs. In 2010, an environmental monitoring program of the municipal waste incineration plant in Barcelona (Catalonia, Spain) was initiated by means of chlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs), polychlorinated biphenyls (PCBs) and polychlorinated naphthalenes (PCNs) by means using passive samplers. In order to establish seasonal and temporal trends, four campaigns (between March 2010 and September 2011) were carried out. PUFs were deployed for 3 months at 8 different locations around the facility. Levels of PCDD/Fs, PCBs, PAHs and PCNs were measured in two different drinking water reservoirs and adjacent drinking water treatment plants in the Czech Republic.

MO 039
L. Vierow, M. Stahl, M. Schlüschner, J.L. Domingo

High-volume active samples have been conventionally used for the environmental monitoring of persistent organic pollutants (POPs) in air. However, these systems have severe limitations, high cost or power inefficiencies. Such passive samplers, being developed, are semi-quantitative measures complementing active systems. Due to the low cost and easy handling, polyurethane foam (PUF) disks are especially attractive. PUFs seem to be a useful tool to compare the state of pollution in specific areas, as well as for seasonal and spatial distributions of local POPs. In 2010, an environmental monitoring program of the municipal waste incineration plant in Barcelona (Catalonia, Spain) was initiated by means of chlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs), polychlorinated biphenyls (PCBs) and polychlorinated naphthalenes (PCNs) by means using passive samplers. In order to establish seasonal and temporal trends, four campaigns (between March 2010 and September 2011) were carried out. PUFs were deployed for 3 months at 8 different locations around the facility. Levels of PCDD/Fs, PCBs, PAHs and PCNs were measured in two different drinking water reservoirs and adjacent drinking water treatment plants in the Czech Republic.

MO 040
L. Vierow, M. Stahl, M. Schlüschner, J.L. Domingo

High-volume active samples have been conventionally used for the environmental monitoring of persistent organic pollutants (POPs) in air. However, these systems have severe limitations, high cost or power inefficiencies. Such passive samplers, being developed, are semi-quantitative measures complementing active systems. Due to the low cost and easy handling, polyurethane foam (PUF) disks are especially attractive. PUFs seem to be a useful tool to compare the state of pollution in specific areas, as well as for seasonal and spatial distributions of local POPs. In 2010, an environmental monitoring program of the municipal waste incineration plant in Barcelona (Catalonia, Spain) was initiated by means of chlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs), polychlorinated biphenyls (PCBs) and polychlorinated naphthalenes (PCNs) by means using passive samplers. In order to establish seasonal and temporal trends, four campaigns (between March 2010 and September 2011) were carried out. PUFs were deployed for 3 months at 8 different locations around the facility. Levels of PCDD/Fs, PCBs, PAHs and PCNs were measured in two different drinking water reservoirs and adjacent drinking water treatment plants in the Czech Republic.
We conclude that CCAFs are an invaluable alternative to conventional air sampling methods, featuring unique advantages, that are a) the exposure estimation of car passengers, riders, pedestrian or road professionals, b) unlimited sample size, ideal for screening of the air quality, especially for compounds that react with particulate on particles, c) provide with an average, time weighted urban air pollution assessment. The main disadvantage of this method is the uncertainty associated with accurate estimations of ambient pollutants concentrations, due to lack of knowledge of the exact amount of air filtered, and the fact that vehicles are used also for trips to less polluted places and/or the fact that also the recirculation of car cabin indoor air is undergoing filtration.
The performance of the new models is presented, methods in a model suite thus allows for a sophisticated consensus modelling of metal bioavailability in sediments from wetlands with different hunting management in Tuscany (Italy).

Determination of these descriptors is tedious and time consuming. Especially for screening purposes, the ability to predict solute descriptors just based on the molecular structure of the tested compound will be beneficial. The commercially available software ABSOLV is an easy accessible and manageable tool that predicts solute descriptors based on a SMILES input. Here we evaluate the performance of ABSOLV to predict partition coefficients using calibrated pp-LFER equations in combination with predicted ABSOLV descriptors. This evaluation is done for various partition processes and a large set of complex, multifunctional organic solutes.

- Different PM and polluted soils (historically polluted and spiked soils); two species of earthworms: L. terrestris (ecologically relevant) and E. fetida (international standard).
- Soil European soils varying widely in physicochemical properties (i.e., pH, organic matter content, texture, eCEC) 
- Toxicity across all seven soils was compared using soils that were amended with Pb and HCl extracted after fresh and aged Pb soils were leached and pH corrected after freshly spiked with lead chloride. This was done to exclude the confounding factors of increased ionic strength and decreased pH due to spiking. Three of these soils (Barcelona, Ter Munck, Woburn) were also amended with lead nitrate in 2004 and aged under field conditions for five years prior to conducting laboratory toxicity tests and additionally tested directly after freshly spiking (without leaching or pH correction). These treatments allow for the estimation of lead ecotoxicity of spiked soils and determination of e.g., correlations between log EC50 and eCEC were highly correlated for the E. fetida reproduction tests, but not for Toxicity of Pb to E. candida was low and not affected by soil properties. Leaching and aging generally attenuated the toxicity of Pb to both soil invertebrates studied. The toxicity data, together with leaching and aging correction factors, provide important information on the bioavailability of lead to invertebrates in soil under realistic conditions.

- Strong influence of particle size and metal speciation on metal bioaccessibility was observed: variation between 20 and 82% according to experimental conditions.
- However, despite of the number of recently published new experimental data, at least to our knowledge there was no relevant new model published within the last years.

MO 046 Lead bioavailability in sediments from wetlands with different hunting management in Tuscany (Italy)

MO 047 Lead bioavailability and bioaccessibility in sediments from wetlands with different hunting management in Tuscany (Italy)

MO 048 Lead bioavailability and bioaccessibility in sediments from wetlands with different hunting management in Tuscany (Italy)

MO 049 Evaluation of a molecular framework based tool for predicting pp-LFER descriptors of complex and multifunctional organic compounds

MO 050 Model suite to estimate the air/water partition coefficient of organic compounds at 25°C

MO 051 EM02P1 - Fate and exposure modelling

MO 052 Lead bioavailability in soil invertebrates as affected by soil physicochemical characteristics

MO 053 E. fetida (international standard for ecotoxicology tests) will be used for laboratory or field experiments. For the different soils before and after bioremediation: i) metal bioavailability will be determined by in vitro UBM test; ii) metal phytoavailability will be assessed by the study of plant uptake (letuce); iii) microscopic (MEB-EDS) and spectrometric (Raman, XRF & Exafs) techniques will be used to perform elementary maps and determine potential changes in metal speciation (cast study); iv) general parameter like survival, biomass changes, cast production and burrowing activities will be studied to assess metal ecotoxicity.

- Strong influence of particle size and metal speciation on metal bioaccessibility was observed: variation between 20 and 82% according to experimental conditions. Moreover significant ecotoxicity effect on earthworm (using cast-production and biomass change measures) was highlighted.
The development of these models was partly supported from the EU Integrated Project OSIRIS (contract No. 037017).

MO 051
ChemProp - chemical properties estimation software system

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The development of ChemProp comprises models to estimate compound properties and a database for chemical structures and properties, together with tools to manage compound sets. The QSPR models for physico-chemical properties with particular remark to partitioning processes of environmental degradation and environmental fate, ecotoxicological endpoints, and human toxicology. It mainly employs models based on the topological matrix and thus does not require quantum chemistry. Particular remark is given to the applicability domain, model uncertainty, and consistency modelling. The integrated database allows for structure and substructure searching, and additionally automated formatting of data. ChemProp is linked to the public OSIRIS ITS webtool (http://osiris.simple.com/OSIRIS-ITS/stixtool.do).

MO 052
Development of a postgraduate course on exposure modeling for environmental risk assessment

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The key strength of the tool is that scenarios can be added for additional geographical areas with relative ease and the appropriate regulatory endpoints. Course materials will be made publicly available.

MO 053
Establishing a postgraduate course on exposure modeling for environmental risk assessment

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Among several multimedia models, the Equilibrium Criterion (EQC) fugacity multimedia model has been widely used for the assessment of the fate, distribution and transport of chemicals in the environment. The model is based on several assumptions to make it representative at a European level but does not necessarily systematically yield realistic exposure estimates. A series of different substances have been chosen differing by their different volatilities and it will be investigating the possibility and feasibility of refining various parameters of the model such as the source description, the emission height and the heat content of the emission plume, suggested by de Bruin et al. (2010). Deposition fluxes in the soil compartment will be calculated on the basis of these refined model parameters and discussed.

MO 054
Parameter reliability in kinetic evaluation of environmental metabolism data - Assessment and the influence of model specification

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Currently, the usual way to determine parameter reliability in kinetic models fitted to environmental metabolism data includes a visual determination, the identification of a relative measurement error level that may explain the residual variance based on a ch2-test and a t-test for significant difference of the parameter from zero. However, the kinetic rate constants can not be smaller than zero and therefore the assumption of a normal distribution is not appropriate. Furthermore, molar formation fractions can only take on values from 0 to 1. Therefore, also in this case a normal distribution can not be assumed. On this poster, several possibilities to overcome these problems are discussed.

MO 055
Development, application, and evaluation of models for screening organic chemical exposures to humans

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Chemicals are being evaluated to protect humans and the environment; however, there are few measured data available for the assessments. For the vast majority of chemicals, mass balance and Quantitative Structure-Activity (Property) Relationship (QSPR) models are required to obtain data on chemical partitioning properties, persistence, bioaccumulation, toxicity (hazard), release rates, exposures to ecological receptors and humans, and risk. Uncertainty in chemical evaluations exists whether the data are measured or modelled and the uncertainty in the measured and predicted data for chemical screening assessments can be substantial. There is a need to address, quantify and ultimately to reduce uncertainty in chemical assessments. The Risk Assessment Identification And Ranking (RAIDAR) mass balance model was used to screen and rank a database of ~13,000 organic chemicals based on far-field human exposure. The model calculations included screening level uncertainty analyses to estimate the propagation of uncertainty in model input parameters on human exposure calculations. Three exposure metrics were selected here: the concentration in a human based on the actual emission rate estimate (CA), the concentration in a human based on an assumed, consistent unit emission rate for all chemicals (CU), and the intake fraction (IF). All of the endpoints are capable of discriminating several orders of magnitude differences in chemical exposure (CA) and exposure potential (iF, CU) are shown to have increasing discriminatory power for screening purposes, increasing biological relevance for human exposure-based prioritization, but sufficiently increasing uncertainty in their calculation due to reliance on additional model input data with high uncertainty (in particular, human, metabolic biotransformation rates and emission rates). Efforts to reduce uncertainty in emissions estimates show reduced uncertainty in exposure estimates in revised screening simulations. The screening results from this holistic exposure assessment method are being evaluated with new and existing (bio)monitoring data and compared with screening results using persistence, bioaccumulation, and ultimate fate and transport models that have been accepted for regulatory assessment in the U.S. and the European Union, including the Pesticide Root Zone Model (versions 3.12.2 and winPRZM 4.51), EXAMS, RICEQW, ADAM (groundwater dilution model), and TOXWA . A key strength of the tool is that scenarios can be added for additional geographical areas with relative ease and the appropriate regulatory endpoints.

MO 056
World exposure assessment tool

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A flexible modelling platform has been developed to evaluate the potential impact of crop protection chemicals on the environment throughout the world. The tool currently has been configured with scenarios containing crop, soil, and weather conditions for major agricultural areas in Canada, Colombia, the European Union, Norway, the People's Republic of China, and the United States. Key processes include using fate and transport models that have been accepted for regulatory assessment in the U.S. and in the European Union, including the Pesticide Root Zone Model (versions 3.12.2 and winPRZM 4.51), EXAMS, RICEQW, ADAM (groundwater dilution model), and TOXWA . A key strength of the tool is that scenarios can be added for additional geographical areas with relative ease and the appropriate regulatory endpoints.

MO 057
Uncertainty analysis using a Fugacity-based multimedia mass balance model: application of the updated EQC Model to D5

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Among several multimedia models, the Equilibrium Criterion (EQC) fugacity multimedia model has been widely used for the assessment of the fate, distribution and transport of chemicals in the environment. The development of these models was partly supported from the EU Integrated Project OSIRIS (contract No. 037017).
of a chemical of interest in the environment. Since the model requires partitioning and reactive properties of the chemical as input data, it is very important to understand how much uncertainties of the physicochemical properties affect the model outcomes. Thus, this study focused on the uncertainty analysis of the EQC Level III model for decamethylcyclopentasiloxane (D5) to quantify the confident range of mass distribution, persistence, and advection, transport rates based on pre-determined dispersion factors of a single source. For the uncertainty analysis, the Monte Carlo simulation technique was employed using Oracle Crystal Ball as an Excel Add-in program to a new spreadsheet platform of the EQC model. The uncertainty analysis showed that once it is released or vaporized to air D5 stays in the compartment until it is removed at a relatively fast rate via OH radical oxidation and water evaporation from the surface. However, D5 is known to be an intermediate transport and non-terrestrial transport and it is not visible to any other compartments. These model outcomes are not virtually affected by the uncertainties of physical properties of D5. On the contrary, when D5 is released to water, a major fraction is distributed in sediment due to sorption of the compound to organic substance in sediment where the degradation rate very small. In this case, the model outcome is predominantly influenced by the uncertainty of KOC. Furthermore, the results of the uncertainty analysis of the EQC model for the scenario (95.5% to 70.8% to water and 4.7% to soil), the 95%-confident ranges of the mass distribution in air and sediment are 47%-78% and 19%-49%, respectively, whereas the overall persistence varies from 3.2 to 5.8 days with the same confidence. The variances are predominantly affected by KOC. Overall, the EQC model results are strongly dependent on the mode of emission. Since the mass distribution in sediment is sensitive to the emission to water, accurate measurement of KOC and 1/3ed is expected to warrant a better understanding of the fate, distribution and transport of D5 in the environment.

MO 058
Multi-scale, multimedia modeling with Pangea - Local to global evaluation of the impacts of a distribution of coal power plants
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Due to a general lack of measured information, predictive methods are required for degradation half-lives in environmental media and in biota to assist in chemical hazard and risk screening. Overall degradability of a chemical in the environment, calculated by the combination of chemical partitioning and environmental media-specific degradation half-lives, is a key determinant of chemical exposure and therefore potential risk. Depending on the partitioning properties, chemical usage, and mode of emission a chemical may be distributed differently in the environment which will alter its overall rate of degradation due to the differential rates of degradation in various physical compartments of the environment (i.e. air, water, soil, sediment). Chemical exposure potential to humans and ecological receptors is also dependent on food web structure, partitioning properties, route of exposure, and differential biotransformation rates of various biota comprising aquatic and terrestrial food webs. In order to interpret the overall degradation on exposure on environmental multimedia multi-pathway mass balance model is required. Using RAIDAR, a multimedia mass balance exposure model linked with aquatic and terrestrial food webs, overall persistence and human and ecological exposures are evaluated as functions of chemical degradability in diverse environmental compartments and organisms. Quantitative structure-activity relationships (QSRAs) are developed to cover as many different environmental media and for the moment it is limited to the distribution of neutral organics. A novel algorithm to develop QSRAs simultaneously for multiple environmental compartments and organisms is applied, and allows for a detailed analysis of the relationship between chemical structural features and exposure potential.

MO 060
Partitioning of organochlorines in storage lipids, membrane lipids and proteins in lean fish
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Lipids are the dominant force in determining organic contaminant accumulation in aquatic organisms because hydrophobic organic chemicals (HOCs) are believed to partition mainly into lipid phase. Therefore, lipid normalized tissue concentrations have been used to reduce variation in tissue residues between different species and aid in understanding toxicity and distribution between different lipids classes. However, partitioning of contaminants between different lipid classes is not very well known. Lipid composition contributes to variation in bioaccumulation potential and neutral storage lipids are thought to be the most important lipid class for HOCs. On the other hand, polar membrane lipids are the target for many HOC toxicity and knowing the concentration in membrane lipids would greatly improve the risk assessment of HOCs. Using D5 as a model lipid for partitioning, we have applied equilibrium partitioning approach to estimate HOC distributions in storage lipid, membrane lipid and protein fractions for carbon 14 labelled PCB-153, PCB-77 and PCB-126. The method is tested with the extracted native PCB contaminated pikeperch oil, and measures of lipid class and protein contents in fish. PCB distribution was dominated by storage lipids (70-78%) while membrane lipids (19-23%) and protein (2-6%) had lower share. The results showed the importance of chemical partitioning to protein fraction in lean fish. The results give new important insight of estimating toxicity using chemical body burden as a dose metric.

MO 061
Simulating ionogenic chemical fate, bioaccumulation and exposure with RAIDAR
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Globally, chemicals are being evaluated for potential hazards and risks to ecological receptors and humans. When measured data are not available, multimedia mass balance models and Quantitative Structure-Activity Relationships (QSRAs) are needed to estimate chemical concentrations in the environment and organisms. Fugacity-based multimedia models and QSRAs are commonly used extensively to accumulation of the environmental load. However, exposure models are limited for ionogenic chemicals. It is estimated that approximately 50% of the 149,000 substances submitted under REACH are ionogenic. The lack of integrated tools for the evaluation of data-poor, ionogenic substances for the complete exposure pathway (i.e. emissions, fate and transport, bioaccumulation in aquatic & terrestrial food chains) reduces confidence in risk assessment for substances with uncertain exposure and toxicological data. The Risk Assessment, Identification And Ranking (RAIDAR) model includes linked fugacity-based multimedia fate and bioaccumulation sub-models, thus providing the capacity to evaluate exposures to humans and ecological receptors in a “holistic” manner. The general objective of this project is to revise and evaluate the RAIDAR model for the simulation of ionogenic chemicals for screening level risk assessment of previously untested chemicals. The model may also be used under data-poor conditions. This presentation outlines the model revisions and explores the fate, bioaccumulation and exposure potential of ionogenic chemicals released to the environment. A hypothetical set of ionogenic chemicals are used to simulate how changes in chemical partitioning properties and dissocation constants affect chemical environmental exposure and uptake rates to different species (i.e. fish, polar and non-polar bird). Simulations are also conducted for current ionogenic chemical of interest in the environment. These simulations highlight data needs for future improvement to model predictions to reduce uncertainty in the assessment of ionogenic chemicals.

MO 062
Predicting the oral uptake efficiency of chemicals in mammals: extension to the hydrophilic range
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Environmental risk assessment requires models to estimate bioaccumulation of untested compounds. So far, most mechanistic bioaccumulation models have focused on very lipophilic compounds, and only few included also more hydrophilic compounds. As shown by pharmacological studies, the membrane permeation of polar compounds is not sufficiently described by octanol/water partition coefficients (KOW). To address this limitation, we adopted a new method to estimate membrane permeability from KOW. Our aim was to develop a model to estimate oral uptake efficiency of pollutants via ingestion in mammals for polar and nonpolar compounds over a wide KOW range of pollutants with focus on polar compounds. The model was based on mechanistic processes and thus included the advective transport of the pollutant through the gastro intestinal tract, the diffusion from the food through the unestered water layer, through the membrane and into the blood. The diffusion through the membrane was split into an inner and outer membrane resistance, where KOW reflected partitioning from the water into the outer membrane, and hydrogen bond donor strength reflected the
partitioning from the outer into the inner membrane. The model was calibrated to two data sets which included uptake efficiency of environmental pollutants measured in different mammals during feeding studies, and a pharmaceutical data set with human oral absorption efficiencies.

A methodology is demonstrated which takes advantage of both GC-MS injection techniques and mass analysis techniques to extend the dynamic range of PAH analysis to encompass these concentrations. This is accomplished while maintaining the required levels of calibration, replicate and sample QA/QC (precision and accuracy), improving the productivity of the laboratory across a wide range of projects.

The development of PAH bioaccumulation in Mytilus galloprovincialis with a three-compartment model

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Polycyclic aromatic hydrocarbons (PAHs) are important organic pollutants in the aquatic environment due to their persistence and accumulation potential both in organisms and in sediments. With the onset of the clean ecosystem, indigenous aquatic biota may be affected due to the accumulation of PAHs in their adipose tissues. These pollutants may occur from primary production in aquatic food chains, starting from primary producers to humans consuming various aquatic organisms with their diet. In this study, mussels were selected as biological indicators due to their broad geographic distribution, immobility and low enzyme activity, which cause significant bioaccumulation of pollutants in their tissues. PAH bioaccumulation and depuration in Mytilus galloprovincialis under dynamic environmental conditions were described using a three-compartment model. First order kinetic equations were used for the description of accumulation and depuration of selected PAHs in mussel tissues. Data were obtained from experiments performed with selected PAHs under constant conditions. In the model, three compartments were defined: (1) mussels, (2) surrounding environment (seawater), and (3) algae (Phaeodactylum tricornutum) as food source for the mussels. During the bioaccumulation period, the mussels take up the contaminants both from seawater and with PAHs sorbed on algae. Thus, the model considers dynamic exchange of PAHs between algae and seawater. Experimental data were used to parameterize and calibrate the proposed model for benzo(a)anthracene and phenanthrene. The observed dynamics could be described well for three different PAH concentrations. The model reflects a mathematical description of bioaccumulation and depuration kinetics of PAHs in mussel species. For better agreement of simulation results with the data, a still a deeper understanding of the processes determining the chemical fate of PAH in the system of seawater, algae and mussels is required.

MO 063
A standardized contact transfer method for assessing soil-to-clothing exposure to soil-sorbed chemicals


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Exposure to chemicals, including chemical warfare agents (CWA), can present a potential Contact Hazard even when the compounds are sorbed onto soil. Previous studies have investigated levels of CWA transferred from contaminated surfaces utilizing a malleable latex material (dentall dam; DD) as transfer substrate; however DD is typically inconsistent in compositions, is not reliable for laboratory investigations. Measurements of CWA on standard Army Uniform (ACU), plus toxicological effects of CWA, have been reliably been established by some CWA and ongoing-testing continues for other; but none still existed for a reliable transfer-exposure method for assessing the exposure potential for chemicals sorbed onto soil. We have established a method for reliably determining Contact Transfer of compounds from soil directly onto clothing, utilizing fabricated swatches (DD) as a standard CWA source to produce transferable concentrations of sorbed mass; then in benchmark investigations, we established the efficacy of CWA extraction from ACU (and DD), and Contact Transfer of CWA from soil onto clothing. A 4" diameter circular swatch of ACU material was selected, similar to surface areas that may contact soil at knee or elbow locations; standard contact was created by placing the ACU swatch directly onto the soil and contact transferred within a minute after transfer was observed. Although ACU transferred increased as a function of contact time, the highest transfer percentage observed was dramatically reduced after 1h; therefore 0.25h was selected for integration into the method. The quantities of CWA transferred from soil surfaces contaminated at operationally important levels from Soil-to-Clothing (ACU) are amounts that are within the range of concern for Soldiers. The standardized Contact Transfer Method provides reliable standard predictions of exposure potential, and in conjunction with toxicity data, for predictions of Contact Hazard.

MO 064
Conjugated modelling of PAH biodegradation, soil sorption and dissolution from organic phases


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Despite promising microbial degradation of polycyclic aromatic hydrocarbons (PAH) in the laboratory, pilot-scale investigations and observations at the field scale often reveal the formation of considerable residual fractions of PAH's on soil, which is not further degraded by microorganisms. The residual PAH fractions result in inconsistent in compositions, and are often due to kinetic reasons, i.e. the concentrations may be too low to maintain microbial metabolism. For a range of biodegradation experiments, combined modelling of microbial growth and microbial degradation, adsorption processes and dissolution from the organic phase has been carried out. The objective of the present study was to analyse and explain observed processes mathematically.

In experiments with phenanthrene solution as model compounds and the degradate monooxidation product 1-hydroxy-phenanthrene, degradation rates of the parent compound were slow, and degradation of the degradate was much faster. It was concluded that the presence of the parent compound was inhibiting the bioavailability of the degradate. A model was developed which takes into account both degradation of the parent compound and degradate, and which allows for the estimation of residual fractions of parent and degradate. The model was successfully verified in a series of degradation experiments using phenanthrene and 1-hydroxy-phenanthrene as parent and degradate, respectively. The model was also used to predict degradation of 2,3,7,8-TCDD and 2,3,4,7,8-HCH in sediments, and to estimate the residual fractions resistant to microbial degradation, which may increase in time. However, residual concentrations may also be due to kinetic reasons, i.e. the concentrations may be too low to maintain microbial metabolism.

The model is being further developed to also include dissolution of compounds from the organic phase. The inclusion of dissolution of the organic phase will allow for a more detailed description of the processes determining the chemical fate of PAH in the system of seawater, algae and mussels. In order to investigate the processes determining the chemical fate of PAH in the system of seawater, algae and mussels, a new dynamic modelling approach (DynANet) based on an existing water-sediment model (DynA) was applied. In DynANet, the implementation of geographic information system (GIS) tools allows the subdivision of a river drainage basin in sub-basins and the resulting river links, classified according to the Strahler stream order, communicate by means of a downstream flow. The loading data of runoff water and modelled chemical concentration coming from the different sub-basins are transferred at each link in the river network. The results of the model were used to study the chemical fate of organic chemicals in the air, litter and soil compartments and working in a GIS environment. The application of the DynANet model to the case study allowed to compile a preliminary mass balance for HHCB and AHTN and to predict concentration changes under environmental phenomena such as precipitations events, temperature variations, soil use, etc. The measured concentrations and simulated results were compared to the prediction of existing models such as GREATER.
MO 068
Estimating chemical emissions from home and personal care products in Asia
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Asia's economy is growing significantly with China and India leading the growth. This has led to an increased demand for home and personal care (HPC) products.

Information on the chemical composition of HPC products and predicted emissions and environmental concentrations (PECs). It has also been demonstrated that by coupling population density data with sales data it is possible to estimate HPC product consumption. To date, most studies have been based in developed markets, where wealth distributions are more homogeneous and HPC products are affordable to all resulting in usage being evenly distributed across the population. In Asia, a population’s wealth and ability to buy HPC products is not uniformly distributed, therefore combining information on population density and sales data with a sub-population’s ability to purchase HPC products could improve chemical emission estimates. Global datasets were sourced for population and economic activity incorporating population, night-time light satellite imagery and land cover. Coupling these datasets with sales data of different HPC products at a (sub) country level and ‘takeoff values’, (a populations ability to purchase products based on their per capita GDP, emission estimates were calculated. Results show large variation in HPC product usage exist across Asia due to the variability in population density and wealth. The largest refinement of emission estimates are associated with products requiring greater purchasing power. As wealth even out, for example the per capita GDP is above $10,000, population density becomes the appropriate method for distributing product use. The potential benefits of this approach include more accurate estimation of chemical emission patterns, which could be used to parameterise exposure models for use in environmental risk assessment and contextualising existing monitoring data.

MO 069
Chemical fate and risk assessment at large scale based on direct and inverse modeling approaches and pan-European datasets
D.T. Marinos1, A. Pistoociochi1, M. Trombetti1, B. Galwik1, G. Bidoglio2
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This work presents the potential of the European version of MAPPE (Multimedia Assessment of Pollutant Pathways in Environment) direct model to simulate a steady-state exchange processes to soils, vegetation and aquatic environments. The geographic distribution of the PCB mixture evolves over time reflecting the sources and sinks' evolvement over time. Therefore, combining information on population density and sales data with a sub-population’s ability to purchase HPC products could improve chemical emission estimates. Global datasets were sourced for population and economic activity incorporating population, night-time light satellite imagery and land cover. Coupling these datasets with sales data of different HPC products at a (sub) country level and ‘takeoff values’, (a populations ability to purchase products based on their per capita GDP, emission estimates were calculated. Results show large variation in HPC product usage exist across Asia due to the variability in population density and wealth. The largest refinement of emission estimates are associated with products requiring greater purchasing power. As wealth even out, for example the per capita GDP is above $10,000, population density becomes the appropriate method for distributing product use. The potential benefits of this approach include more accurate estimation of chemical emission patterns, which could be used to parameterise exposure models for use in environmental risk assessment and contextualising existing monitoring data.

MO 070
Multimedia assessment of chemical exposure by MAPPE-Global explicit model: a case study of pollutant discharge to Mediterranean Sea
EC, JRC, IES, Ispra, Italy
Global fractionation of PCBs are ubiquitous environmental pollutants which are expected to decline in abiotic environmental media in response to decre

PCBs are ubiquitous environmental pollutants which are expected to decline in abiotic environmental media in response to decre

 Destruction; advective transport; diffusive transport; and sinking. The results suggest that the effectiveness of emission control measures may significantly vary among substances, not only reflected as latitudinal gradients, but also as longitudinal gradients.

MO 071
The impact of including ice and snow in multicompartmental modelling of persistent organic pollutants' distributions and fate
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3University of Milano-Bicocca, Italy
The study encouraged the applicability of the inverse modeling technique for pollutants with poor and sparse emission estimates but which were extensively monitored in environmental samples. An example the capability of the inverse GIS applications was utilised for backward tracking of PFOA and PFOA emission factors from riverine measurements and to investigate the loading of the widely used pharmaceuticals and personal care products to European rivers.

MO 072
Chemical fate and risk assessment at large scale based on direct and inverse modeling approaches and pan-European datasets
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The impact of including ice and snow in multicompartmental modelling of persistent organic pollutants' distributions and fate

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The results suggest that the effectiveness of emission control measures may significantly vary among substances, not only reflected as latitudinal gradients, but also as longitudinal gradients.

MO 073
The impact of including ice and snow in multicompartmental modelling of persistent organic pollutants' distributions and fate
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The impact of including ice and snow in multicompartmental modelling of persistent organic pollutants' distributions and fate

Global fractionation of PCBs are ubiquitous environmental pollutants which are expected to decline in abiotic environmental media in response to decre

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MO 074
Global environmental cycling of DDT and gamma-HCH in the 1980s - a study using a coupled atmosphere and ocean general circulation model
T. Marinov1, A. Pistocchi2, M. Trombetti3, B. Galwik3, G. Bidoglio3
1EC, JRC, IES, Ispra, Italy
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MO 073 Uncertainty analyses with Monte Carlo simulation determined that hydrolysis half-life in water and sediment layer depth was the most influential input parameter to the modelled fate of D5. The residence time of D5 in water was relatively short compared to that in sediment.

MO 074 Environmental fate, latitudinal distribution and long range transport of decamethylcyclopentasiloxane (D5) in the global environment: a model assessment

S. Xu, E.W. Wania

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Decamethylcyclopentasiloxane (D5) is widely used as an ingredient in the formulation of personal care products, or is present as an impurity in the silicone fluids and rubbers. The global environmental fate, latitudinal distribution, and long range transport of D5 was analyzed by two multimedia chemical fate models using the best available physicochemical properties as inputs and known persistent organic pollutants (POPs) as reference. The global transport and accumulation characteristics of D5 differ from those of typical POPs in three significant ways. First, a large fraction of the released D5 tends to become airborne and is removed from the global environment by degradation processes. This is in contrast to the fate of typical POPs, where a small fraction of the released compounds is transformed to larger chemical moieties and transported to remote regions. Second, D5 shows a much lower bioaccumulation potential, toxicity and ubiquitous presence in the natural environment compared to typical POPs.

MO 075 Assessing and comparing the influences of uncertainty in chemical property data and variability in climate variables on the simulated fate of PCBs

K. Dugué, L. Zhe, M. Matthew, C. T. Iannone

Stockholm University, Stockholm, Sweden

Leveraging chemical property data (POPs) are of concern due to their persistence, bioaccumulation potential, toxicity and ubiquitous presence in the natural environment. Environmental fate modellers have made numerous efforts to simulate the transport and fate of legacy POPs at different spatial and temporal scales. The success of modelling exercises depends largely on the quality of input data for characterizing either the modelled chemicals or the modelled environment, e.g. the physical-chemical properties and environmental (including climate) variables. The purpose of this study is to explicitly assess and compare the influences which are caused by the uncertainty in chemical property data and variability in climate variables. Representative polychlorinated biphenyl (PCB) congeners having a range of physical-chemical properties are selected as study chemicals. The scientific literature was mined to describe the uncertainty in the physical-chemical properties of the selected PCBs, and online climate databases were used to estimate the long term average, interannual and interdecadal deviations of typical climate variables. The final uncertainty analysis was performed for Japan and used to test the hypothesis that property uncertainty has more influence on model outcomes than climate variability. The robust statistical tool Oracle® Crystal Ball (Fusion edition, 11.1.1.1.0) is adopted to perform the correlation and sensitivity analyses. Generally speaking, results suggest that uncertainty in physical-chemical property data, i.e., more pronounced variances in the model predictions than variability in climate variables, i.e., the predicted environmental fate and distribution of selected PCB congeners is more sensitive to uncertain physical-chemical properties than to climate variables. The large uncertainties associated with half-lives for degradation in air, water and soil dominate influences on the model simulated fate and distribution of selected PCBs, if compared to climate variables and the physical-chemical properties. Among climate variables, temperature and its projected future deviations is the most influential. We conclude that predicting the influence of climate on chemical transport and fate is challenging due to the fact that climate-related effects on transport and fate are relatively small compared to uncertainties in physical-chemical properties and degradation rates.

MO 076 Environmental fate of D5 Predicted by the QWASI Fugacity model

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The QWASI fugacity model predicted that when D5 is released to water, multiple processes including volatilization, sorption to sediment, advection and hydrolysis take place competitively. Importantly, the rates of transport and transformation processes are dependent on the local aquatic environment. Since a better quantitative assessment on the fate, distribution and transport of D5 in the local water body system is needed, this study evaluated the environmental behavior of D5 in Lake Ontario (LO) and Lake Pepin (LP) at various environmental temperatures and under steady-state and unsteady-state conditions. Additionally, uncertainty analyses were performed to determine the most probable range of the model outcome and the most influential input parameters using a new Quantitative Water Air Sediment Interaction (QWASI)-Excel model. The QWASI-Excel model predicted that water concentration of D5 decreased for both lakes due to increase in hydrolysis rate with rising temperatures from 1 to 25°C. In contrast, D5 concentration profiles in sediment were different: it decreased gradually from 1.0 to 0.5 ng/g dw in LO whereas it increased from 120 to 280 ng/g dw in LP. D5 mass preferentially distributed to water in LO but to sediment in LP. Mass fraction of D5 increased with temperature for both lakes mainly due to increased Koc value. D5 was removed from air through different pathways and adsorption to sediment and plants was a function of layer in the canopy. The model also includes a new wet deposition scheme that estimates the interception of gases dissolved in rain as a function of depth in the canopy.

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1Dow Corning Corporation, Auburn, Michigan, United States of America

Decamethylcyclopentasiloxane (D5) is widely used as an ingredient in the formulation of personal care products, or is present as an impurity in the silicone fluids and rubbers. The global environmental fate, latitudinal distribution, and long range transport of D5 was analyzed by two multimedia chemical fate models using the best available physicochemical properties as inputs and known persistent organic pollutants (POPs) as reference. The global transport and accumulation characteristics of D5 differ from those of typical POPs in three significant ways. First, a large fraction of the released D5 tends to become airborne and is removed from the global environment by degradation processes. This is in contrast to the fate of typical POPs, where a small fraction of the released compounds is transformed to larger chemical moieties and transported to remote regions. Second, D5 shows a much lower bioaccumulation potential, toxicity and ubiquitous presence in the natural environment compared to typical POPs.

MO 078 Modelling aluminium fate and transport in ground and surface water for Life Cycle Assessment

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In assessment of the fate, transport, and ultimate exposure of metals to humans, correctly accounting for long-term groundwater emissions, e.g., from a landfill, has been challenged. This paper offers a new perspective on human exposure to anthropogenic metal emissions to ground and surface water. Existing models, such as the Ecoinvent LCA database have assumed 100% of landfill emissions reach surface water. To accurately reflect geochemical and hydrologic processes, this conservative assumption can be reassessed.

A multimedia component model was developed to assess the total intake by humans of emissions to landfills (for aluminium) and directly to surface water (for arsenic from aluminium ore). For aluminium emissions, a kinetic precipitation model was developed to estimate transfer to surface water. In surface water, the geochemical model PHREEQC is used to model aluminium fate and transport in ground and surface water.
A study of the relevance of regionalization and archetype approach for aquatic freshwater ecotoxicity

MO 079

Dioxin Source to Ecological Region HypSPLIT-SV Modeling in Arctic with Metropolitan Achievements 2008-2010: Montes Azules, Celestun and Monterrey


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Instituto Nacional de Ecología., Mexico d.f., Mexico

NGO, Global 2000, United States of America

Instituto Nacional de Ecología (INE) sampled and measured dioxin in the atmosphere at 10 research stations in Mexico from 2008-2010 with the support of the U.S. Environmental Protection Agency, Environment Canada, Health Canada, and the Commission for Environmental Cooperation for North America. We focus in this presentation on receptor regions with air mass models that need to be calibrated and the results are: in good agreement with receptor regions, lands., Celestun (ecosensitive biodiverse ecoservice, land and marine), and Monterrey (urban and agricultural). The Hybrid Single Particle Lagrangian Integrated Trajectory Semi-Volatile experimental research atmospheric dispersion model (HYSPLIT-SV) is employed to account for variations from meteorology under conditions of uncertain source emissions.

HYSPLIT-SV is a dynamic atmospheric dispersion model adapted to include atmospheric chemistry and environmental fate processes involving vapor-particle partitioning, degradation (e.g. via hydroxyl radical, ozone, photolysis) and deposition (wet and dry; gas and particle). Source-to-receptor simulations produce estimates of the efficiency of source-to-receptor transport for exposure characterization factors for freshwater ecotoxicity. The water mass model in each receptor region was important in the contribution of the fate factors of dioxins ranging from the atmospheric to the riverine receptors.

The importance of regionalization for the aquatic freshwater ecotoxicity impact category has been evaluated at different resolutions (at a watershed, country and continental scale) using multimedia fate and exposure models such as IMPACT World, Europe single zone and Europe spatial models. A first comparison of water fate factors between the IMPACT European spatial model vs. the IMPACT European spatial model has been performed considering both a uniform emissions and emissions in each specific watershed. Moreover three watersheds with short, medium and high residence time of water to the sea have been selected to analyze the importance of chemical properties vs. watershed specific properties to identify the key parameter(s) influencing the fate. The water residence time was used as the basis for defining 2 watershed archetypes, i.e. upstream (water residence time >0.1 [yr]) and downstream of a lake (water residence time <0.1 [yr]). The fate factors of dioxins in each archetype and the target water quality data. The applicability of this model as decision making tool for pollution control activities was also assessed and the result is encouraging.

Recommendation, which takes into account the existing water quality problem in the study area, has been suggested for improvement and wider application the model.

MO 081

Mathematical modeling of point source pollutants fate and transport in the Little Akaki River, Ethiopia

T.N. Hamdi

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Computer models are becoming increasingly important tools in every environmental management aspects. A general one-dimensional water quality model has been developed for one of the most industrially concentrated and polluted rivers in Ethiopia - the Little Akaki River. The study covers a total of 27.4 km length along the river where pollution issues have been recorded for the spatial and seasonal periods. The water geometry and hydrometeorological data were collected from various locations along the river. A first comparison of water fate factors between the IMPACT Europe single zone and Europe spatial models is important in the contribution of the fate factors of dioxins ranging from the atmospheric to the riverine receptors.

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Recommendation, which takes into account the existing water quality problem in the study area, has been suggested for improvement and wider application the model.

MO 082

Mixing zones modeling in the water framework directive: comparison between “discharge test” and 'CORMIX'

M. Eliot, P. A. J. Van-Speybroeck, ARCHE, Gent, Belgium

The Priority substance Directive 2008/105/EC has defined EQS for 33 priority substances. Compliance with these EQSs should be achieved at the point of discharge or at least at the outfall of the receptor. To achieve this the receptor model has been developed to assess the compliance with the EQS values. The approach starts with simple investigations but could end with very detailed assessments on the mixing behavior and concentration profile of effluents in the surface waters. In contrast to lower tiers, higher tiers require an estimate of the extent of EQS exceedence that can be used to define a mixing zone. This may be achieved using a full water mass model and the spatially differentiated model for unknown emission location (i.e. assumed being uniformly emitted compared over the whole model surface).

When the emission location is known, a spatially differentiated model can improve the model accuracy up to 2-3 orders of magnitude, because of its ability to accurately predict the water residence time to the sea (or out of the system) depending on the emission location. Is therefore spatial differentiation always required? The answer depends on the specific property of the chemical: only for persistent chemicals the water residence time plays a key role in determining the chemical fate for freshwater ecosystems. Highly degradable or volatile chemicals for example would disappear before being advected out of the system. This support that, for persistent chemicals, the country regional differentiation is relevant.

MO 083

Developments of GREAT 3.0: an entirely Open Source software for river and sediment exposure modeling

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GREAT (Geography-referenced Regional Exposure Assessment Tool for European Rivers) is a GIS-assisted computer model for risk assessment and management of chemicals in river basins. Since the release by ECETOC of the original model in 1999 (GREAT 1.0) a number of regional projects have been initiated by various organizations with the aim of exploring and expanding the different applications of the model.

To facilitate this process, the model system was reimplemented with a modular architecture and a database back-end in 2003 (GREAT 3.0 Desktop and GREAT 3.0 Web).
Over the years, the GREAT-ER model has served a worldwide user community, and currently more than 170 different scientific papers refer to the development or application of the model. Under the sponsorship of the CEFIC-LRI programme, the package has now been updated again as GREAT-ER 3.0 (2011). Most notably, the database has been replaced by the Open Environmental Security (OES) database without any software licence fee, and the scientific community is welcome to analyse and use the Freeware GREAT-ER. On the model side, GREAT-ER 3.0 now also includes a sediment extension, and the possibility to model lakes as part of a river basin.

Information on GREAT-ER and updates on different projects initiatives can be found at www.great-er.org.

MO 084
Case study using the tiered approach for mixing zone modeling in the water framework directive
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ARCHE, Gent, Belgium

The priority substance Directive 2008/105/EC has defined EQSs for 33 priority substances. Compliance with these EQSs should be achieved at the point of discharge or at least at the edge of the mixing zone in the receiving waters. Considering this, a “Tiered Approach” has been developed to assess whether compliance with the EQS values is achieved. The approach starts with simple investigations but could end with very detailed assessments on the mixing behavior and concentration profile of effluents in the surface discharges. For higher tiers, more intensive investigations of the extent of EQS exceedance that should be used to define a mixing zone. This may be achieved using a range of tools such as “Discharge Test” or “CORMIX”. The aim of this poster is to present a test case using the tiered approach. An industrial site has a surface discharge with a flow rate of 1,000 m³/d to a small river characterized by a flow rate of 18,000 m³/d. Concentration of the contaminant of concern in the effluent ([CoCl₄]₃) is 30 µg/L which is higher than the EQS of the CoCl₄ with an EQS is present in the effluent and the [CoCl₄]₃ > EQS therefore triggering the initiation of the second tier. The Process Contribution (PC) is 2.63 µg/L representing 13% of the EQS after complete mixing. This is higher than the allowed 4% and therefore higher tiers should be initiated and an estimation of the extent of the mixing zone is required. Surface discharges are best modeled with CORMIX requiring the discharge characteristics, sedimentary input, and receiving water. Due to the importance of the near field interactions, both the geometry and position of the discharge has to be well defined. In this case study, the discharge is located on the left bank pointing perpendicular to the river with a local depth at discharge of 0.4 m and a slope of 5 degree. The discharge channel is 0.3 m wide and 0.3 m deep. CORMIX simulations show that at approximately 0.6 m downstream of the discharge point the [CoCl₄]₃ drops below the EQS. A proposed extend of the mixing zone is described in the example EQS which in the test case would be 20 m. Therefore the CoCl₄ will be below the EQS in the proposed mixing zone of 20 m and compliance is achieved.

MO 085
Source apportionment of chemicals under the WFD
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³BPP, London, United Kingdom

New Environmental Quality Standards (EQS) are being set under the Water Framework Directive (WFD) for a wide range of substances. Generally, the concentrations for these EQS are lower than existing values. However, the sources of many of these substances are wide ranging, particularly for metals and nutrients, with multiple diffuse and point source inputs into the aquatic environment. Where an EQS is exceeded, Programmes of Measures (PoMs) may be required to reduce inputs to the aquatic environment subseptating the attainment of technical feasibility and disproportionate costs. The WFD states that compliance should, as a priority, be achieved via source control, applying the ‘polluter pays principle’. To apply effective PoMs it is therefore necessary to accurately quantify sources of chemicals discharged to the environment. A review of available databases has demonstrated that there are no available national scale source apportionment models. UK Water Industry Research (UKWIR) in collaboration with the Environment Agency has therefore developed the GREAT-ER model into a national scale source apportionment tool. The EPA funded the development of a model of future river basin planning. The model has been calibrated using available data. With the availability of national EQS values, the GREAT-ER model is now being used to perform national scale source apportionment for metals and nutrients, and in the future inorganic and organic substances. The UKWIR model has also been used by the GREAT-ER model for national scale source apportionment models for metals and nutrients. The GREAT-ER model was used to define a mixing zone. This may be achieved using a range of tools such as “Discharge Test” or “CORMIX”. The aim of this poster is to present a test case using the tiered approach. An industrial site has a surface discharge with a flow rate of 1,000 m³/d to a small river characterized by a flow rate of 18,000 m³/d. Concentration of the contaminant of concern in the effluent ([CoCl₄]₃) is 30 µg/L which is higher than the EQS of the CoCl₄ with an EQS is present in the effluent and the [CoCl₄]₃ > EQS therefore triggering the initiation of the second tier. The Process Contribution (PC) is 2.63 µg/L representing 13% of the EQS after complete mixing. This is higher than the allowed 4% and therefore higher tiers should be initiated and an estimation of the extent of the mixing zone is required. Surface discharges are best modeled with CORMIX requiring the discharge characteristics, sedimentary input, and receiving water. Due to the importance of the near field interactions, both the geometry and position of the discharge has to be well defined. In this case study, the discharge is located on the left bank pointing perpendicular to the river with a local depth at discharge of 0.4 m and a slope of 5 degree. The discharge channel is 0.3 m wide and 0.3 m deep. CORMIX simulations show that at approximately 0.6 m downstream of the discharge point the [CoCl₄]₃ drops below the EQS. A proposed extend of the mixing zone is described in the example EQS which in the test case would be 20 m. Therefore the CoCl₄ will be below the EQS in the proposed mixing zone of 20 m and compliance is achieved.

MO 086
Persistence of petroleum hydrocarbons in seawater: modeling versus experimental results
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Hydrocarbons are a highly reduced form of carbon which provides a valuable source of energy for microorganisms. Therefore, mechanisms have evolved to degrade them, and nearly all hydrocarbons can be degraded under appropriate conditions. However, degradation of petroleum hydrocarbons in biodegradation studies is often underestimated, mainly due to the physical and chemical properties of these substances. One of these properties is their low water solubility, which results in low bioavailability to microorganisms. Biodegradation data are required by many regulatory frameworks around the world. In the persistence assessment for petroleum substances under the EU REACH regulation, biodegradation data for the major hydrocarbon classes present in these substances were used. In order to screen for persistence, aquatic half-life predictions for representative compounds were calculated using the BioHCwin module of the EPISuite v4.0 model. These predictions allowed narrowing the range of potentially persistent hydrocarbon classes and carbon classes, thereby optimizing biodegradation testing efforts. To experimentally test biodegradation for the hydrocarbons of interest, a new experimental methodology was used which determined single hydrocarbon biodegradation in seawater. To prevent variability due to water quality constraints, a passive dosing system, designed to simulate the near field of a point source, was used to load the seawater with the chosen hydrocarbons. Biodegradation was measured using a respirometer, which performed automated dissolved oxygen measurements in the test vessels and minimized variability due to experimental handling. Except for highly branched structures or structures with quaternary carbons, experimental results showed that in general, seawater biodegradation model predictions were overly conservative. It can be concluded that the combination of modeling results and targeted experimental data provided a complete and robust assessment of the persistence of petroleum hydrocarbons.

MO 087
Field to continental phosphorus fate and eutrophication modelling
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To date, it has been difficult to link agriculture practices with local, regional, and long-distance impacts. Using a milk-producing farm as an example, this work demonstrates the possibility for improved environmental impact analysis based on the integration of site-specific biogeochemical models, local hydrology data, and fate and impact models, linking these from the local to regional scale. An existing model [Manure-DNDC] [1] was extended to include phosphorus (P), and a new, global P transport model was developed. Based on site-specific information, the Manure-DNDC model calculates total phosphorus loss from the milk producing farm. Subsequently, watershed specific data is used to estimate the amount of P that reaches the local stream. Once the load is distributed to local streams, it is routed downstream using a newly developed approach [2] that incorporates advective transport, deposition in waterways due to physical settling and biological uptake, and removal from the water system due to water withdrawal. The environmental impact of these incremental phosphorus additions can be assessed by comparison to existing phosphorus concentrations.

Manure-DNDC was used to simulate the runoff flow, sediment yield, and P loads for two test farms. Predictions showed agreement with validation data within a factor of two, and always within one order of magnitude. The model predictions of the fate of emitted phosphorus show that total ecosystem impact, and the location of that impact, is strongly dependent on the location of emission. In the case of the emission to the Great Lakes, the long residence time of water means that the majority of impacts can occur within 200 km of the point of emission, depending on whether impacts are assumed to occur at all existing P concentrations or whether there is a threshold value. For emissions in the Mississippi watershed, ~25% of impacts occur within 50 km; ~45% occur between 50 and 200 km, and ~30% occur greater than 200 km away.


MO 088
ENM fate in freshwater through adaption of USEtox (tm)
M.M. Missetlíc, S.L. Olsen, M. Birked

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Engineered nanomaterials (ENMs) have in recent years received substantial attention, both in scientific and consumer circles, as these materials are introduced to a steadily increasing number of consumer products. This has led to environmental concerns on how this new material class behaves in the environment, at which concentrations
organisms are exposed to the materials and what effects these materials may have on the environment. In relation to metal-oxide engineered nanomaterials (ENMs), as is the case for ENMs, many environmental aspects are still unknown and/or not properly scientifically mapped. One approach that has not been given much attention in relation to environmental assessment of ENMs, more precisely the fate, exposure and effect modelling of metal-oxide ENMs is the application of adapted characterisation models designed for single [chemical] compound assessment e.g. the USEtoX model for characterisation of ENM effect potentials.

The purpose of this study is therefore to evaluate if existing characterisation model such as the USEtoX model can be applied for characterisation modelling of ENMs applying single [chemical] compound assessment. The primary advantage of the adapted characterisation relies on the recognition of the fact that nano-materials do not behave like simple chemical compounds in the environment. The second principle of ACM relies on the fact that existing chemical characterisation can be applied to model hypothetical representatives for effect causing emissions such as groups of chemicals (i.e. equivalence approaches applied to model mercury). In this study the approach taken was therefore to consider the fate of EF and appropriate valid. The characterisation was done by relating nano-material properties to chemical properties and hence model the nano-material as a chemical with representative fate and exposure patterns.

In the case study involatile ENM's [metal-oxides] were characterised in USEtoX applying adapted characterisation modelling. The result obtained indicates that with some limitations the approach is considered valid - the characterisation factors are considered uncertain relating to several facts such as lack of environmental studies on ENMs making is hard to assess the general environmental behaviour of ENMs and hence relate this environmental behaviour to similar "chemical behaviour".

**MO 089**

Use of multiple tracers to assess non-stationarity of hydrologic transport at the catchment scale

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Abstract

The aim of this study is to estimate chemical concentrations in river compartments using a 1D numerical model for contaminant transport. The variability of the heterogeneity of the catchment zone (soil properties, preferential flowpaths, evaportranspiration losses, etc.) acting as a stochastic hydrologic filter suggest non-stationary solute travel time distributions. Several travel-time based models have already been developed, but experimental validation is still lacking for this type of models. In order to establish experimental travel-time distributions, 1) temporally displaced tracer injections and 2) spatially displaced tracer injections are conducted in the hillslope of the Chamberonne river (Lausanne, Switzerland). Tracer concentrations are measured downstream both close from the injection site and at the catchment outlet in lake Geneva. In the first experiment, pulse loads of different tracers are injected at the same spot nearby the stream, in order to emphasise the effect of antecedent soil-water conditions resulting from climatic forcing and hydrologic filtering. The extent of the soil water deficit is the main trigger of non-stationarity in the arrival-time distributions. In the second experiment, pulse loads of different tracers are injected at different locations of the stream varying between 5 and 50 meters. In this case, simultaneous injections are emphasising the effect of heterogeneity in the hydrological pathways under similar soil-water conditions. In both experiments, the use of multiple tracers analytically differentiable is essential in order to be able to identify the original time and location of the tracer injection. This allows to physically measure the influence of the sequence of precipitations and soil heterogeneity on solute transport travel time.

**MO 090**

Estimation of chemical concentrations in river compartments using a 1D numerical model for contaminant transport

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Abstract

In this study, the use of multiple conservative tracers is proposed in order to calculate the arrival time distributions of a solute through hydrologic transport. The variability of the heterogeneity of the catchment zone (soil properties, preferential flowpaths, evaportranspiration losses, etc.) acting as a stochastic hydrologic filter suggest non-stationary solute travel time distributions. Several travel-time based models have already been developed, but experimental validation is still lacking for this type of models. In order to establish experimental travel-time distributions, 1) temporally displaced tracer injections and 2) spatially displaced tracer injections are conducted in the hillslope of the Chamberonne river (Lausanne, Switzerland). Tracer concentrations are measured downstream both close from the injection site and at the catchment outlet in lake Geneva. In the first experiment, pulse loads of different tracers are injected at the same spot nearby the stream, in order to emphasise the effect of antecedent soil-water conditions resulting from climatic forcing and hydrologic filtering. The extent of the soil water deficit is the main trigger of non-stationarity in the arrival-time distributions. In the second experiment, pulse loads of different tracers are injected at different locations of the stream varying between 5 and 50 meters. In this case, simultaneous injections are emphasising the effect of heterogeneity in the hydrological pathways under similar soil-water conditions. In both experiments, the use of multiple tracers analytically differentiable is essential in order to be able to identify the original time and location of the tracer injection. This allows to physically measure the influence of the sequence of precipitations and soil heterogeneity on solute transport travel time.

**MO 091**

In situ characterization of metal-oxide engineered nanomaterials for effect assessment in mountainous regions

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Abstract

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**MO 092**

Bioaccessibility options for detailed quantitative assessment of metals

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Abstract

The need for a rapid risk assessment approach for the assessment of contaminated land and human health impact is becoming more apparent. As part of this approach, Soil Guideline Values (SGV) and Generic Assessment Criteria (GAC) have been developed to enable Generic Quantitative Risk Assessment (GQRA). One of the main assumptions in the derivation of these criteria is that 100% of the contaminant present in the soil will be bioavailable or bioaccessible. Whilst this assumption may be necessary in the preliminary stages of risk assessment to ensure the protection of human receptors, it may result in overly conservative risk assessment. Recommendations for remediation may subsequently be made in situations where remediation is not appropriate.

Recent years the potential for bioaccessibility data to be incorporated into Detailed Quantitative Risk Assessment (DQRA) has been increasingly recognised. To investigate the potential for the application of bioaccessibility data in DQRA, GAC for bioavailable metals based on the contaminated Land Exposure Assessment model (CLEA) have been derived for selected metals; arsenic, cadmium, mercury, nickel and vanadium for standard residential, commercial and allotment land use. By comparing GACbio to typical contaminant concentrations encountered in UK soils we explore the options for the future application of bioaccessibility data.

A risk evaluation of the need to remediate based on the use of literature estimates of bioavailability or of GAC that invoke generic bioavailability values would be difficult to defend. GACbio however can be useful in determining whether to incur the cost of site specific studies of bioavailability. The applicability of GACbio can be determined by contrasting three lines of evidence: history of contaminant formation (natural or anthropogenic); geochemical sequential extraction and physiological based tests. The natural or anthropogenic geochemical processes that led to the contamination and the formation and current disposition of the contaminants of concern (CoC) at a specific site will give an indication of the likely chemical instability and therefore bioavailability of such CoC. Sequential extraction testing can give an indication of the mineral species with which different fractions of the CoC are associated and hence their likely availability. Finally empirical physiologically based tests can give an insight into the material specific chemistry. 

**MO 093**

Urban versus rural GIS-based distinction for human health impacts in LCA. Application on automotive fuels

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Life cycle assessment (LCA) is frequently used to assess the sustainability of the various alternative fuels that are emerging. However, local impacts, especially human health (HH), are often neglected. This is because they are heavily dependent on the local context and thus difficult to understand. In this study, we introduce two distinctions in order to improve HH impacts in LCA of alternative fuels: urban versus rural and high versus near-ground emissions.
The mathematical simulation model SiMBaFi was developed in a project to replace the multiplier on adsorption and degradation in a water environment. It is then coupled with USEtox to distinguish between urban and regional emissions. This was coupled with ReCiPe methodology, allowing differentiating between urban and rural emissions. The EU and national registration processes require the assessment of the leaching potential of an active ingredient and its metabolite(s) of plant protection products (PPP) to groundwater as described in the FOCUS Groundwater reports (2000 and 2009). For groundwater simulations using FOCUS-PELMO 4.4.3 in the framework of the national registration procedure in Germany, new recommendations related to Tier 1 and Tier 2 were published by the Federal Environment Agency (UBA) and the German Agrochemical Industry Association (IVA) (Holdt et al. 2011). Input Decision 3.1, an easy to handle MS Excel-tool, was developed to select sorption endpoints for realistic worst case groundwater modelling considering a relationship between sorption behaviour and soil properties and for the selection of DT50-values linked to the recommendation to apply one or two suitable scenario(s) in FOCUS-PELMO 4.4.3 simulation relevant for the German groundwater assessment. The approach presented here may contribute to a harmonisation of exposure assessment for PPP between national, zonal and European level in future.

MO 094
A new version of input decision for the selection of modelling endpoints for PEC gw simulations for harmonisation of exposure assessment

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The EU and national registration processes require the assessment of the leaching potential of an active ingredient and its metabolite(s) of plant protection products (PPP) to groundwater as described in the FOCUS Groundwater reports (2000 and 2009). For groundwater simulations using FOCUS-PELMO 4.4.3 in the framework of the national registration procedure in Germany, new recommendations related to Tier 1 and Tier 2 were published by the Federal Environment Agency (UBA) and the German Agrochemical Industry Association (IVA) (Holdt et al. 2011). Input Decision 3.1, an easy to handle MS Excel-tool, was developed to select sorption endpoints for realistic worst case groundwater modelling considering a relationship between sorption behaviour and soil properties and for the selection of DT50-values linked to the recommendation to apply one or two suitable scenario(s) in FOCUS-PELMO 4.4.3 simulation relevant for the German groundwater assessment. The approach presented here may contribute to a harmonisation of exposure assessment for PPP between national, zonal and European level in future.

MO 095
Estimation of soil moisture and temperature based on different soil hydraulic pedotransfer functions

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The time-step normalisation procedure as described by FOCUS (2006) can be used to normalise soil field dissipation rates and to derive DT50 value standardised to 20°C and pH 7. This normalisation procedure decreases or increases individual day lengths by means of daily correction factors based on soil moisture and soil temperature. Hence, soil properties such as moisture and temperature also need to be available in daily resolution. For many soil dissipation studies in the field, these parameters are, however, not available. We applied or still run a realistic assessment, average daily soil moisture and temperature values can be estimated with predictive models, e.g. PEARL. For the present assessment, Van Genuchten parameters are derived from the soil properties of a trial site located in Central Europe. Therefore, three different types of soil hydraulic pedotransfer functions are tested. The respective results will be compared to measured soil conditions to determine a simulation method that represents realistic field conditions. Climate data (mean/minimum temperature, precipitation, global radiation) are from the respective time period of the study. Additionally, measured soil moisture (10 cm depth) and soil temperature values (5 cm and 20 cm depth) for 12 data points were available, respectively. Hydraulic pedotransfer functions were prepared based on the HYPRES database (Nemes et al. 2001), the Rosetta database (USD 2000) as well as the Staring Series (Wösten et al. 1994, Van Genuchten 1980). For each approach a specific PEARL scenario was created using the corresponding Van Genuchten parameters. For the PEARL simulations a soil profile of 1 m depth were defined. The profile consisted of five horizons (20 cm each). Soil characteristics were only available for the uppermost horizon (0 - 20 cm) and they were duplicated to be identical in all horizons. The PEARL soil moisture and soil temperature simulations were evaluated for the first horizon (0 - 20 cm) for different depths steps (1 cm resolution). The simulated daily soil moisture and soil temperature data from the respective depths were compared to soil moisture and soil temperature measurements from samplers. For the PEARL parameterisation a goodness of fit indicator (sum of squared errors between simulated and estimated volumetric soil moisture), the estimation method that represents measured data from the trial site the best will be determined.

MO 096
Bank filtration simulation model SiMBaFi - a tool to refine the PEGroundwater as part of the environmental risk assessment of medicinal products for human use

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In Phase II Tier A of this guideline the potential entry of a pharmaceutical into the groundwater (PEC groundwater) by bank filtration is calculated by multiplying the predicted environmental concentration of surface water (PEC surfacewater) by a factor of 0.25. This factor does not consider substance specific properties, or originated by expert judgment. The bank filtration simulation model SiMBaFi was developed in a project to replace the multiplier (0.25) by a model based decision matrix taking into account the following parameters: distance between shore line and extraction well, depth of filter screen, hydraulic conductivity and average extraction rates. The result was a Microsoft Access application which calculates the PEC groundwater for 3 standard flow times scenarios (worst case = 0.15 d, realistic worst case = 5 d, median case = 100 d). The following substance properties are needed as input parameters to determine the concentration in groundwater: sorption coefficient (Kd) and degradation (Dt50). This poster will present the results of groundwater exposure calculations with SiMBaFi for more than 30 pharmaceutical ingredients for which experimental data on adsorption and degradation in a water-sediment system were available. The comparison with the multiplier allows a first assessment if an implementation in the environmental risk assessment as groundwater exposure tool is useful.

MO 097
Biodegradation in heterogeneous soils: reactive transport of active substances revisited

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The heterogeneity in soils is influenced by its texture, density, porosity, and the distribution and state of microbial life. Soil physical properties as well as microbial life have an impact on the fate of active substances in the soil environment. Microorganisms occur in soil pores either in suspension or as biofilms which alter the pore geometry which in turn alters the residence time. This alteration directly influences the soil water flow field and hence the convective transport of organic substances. Furthermore, the activity field of microorganisms degrading those substances depends on soil properties. We will present an upscaled model which combines spatial stochastic generation of soil structures at pore scale and a process model at column scale coupling fluid flow, reactive transport, and biofilm dynamics. Process models are formulated by a system of coupled partial differential equations which is solved by a Petov Gekker scheme (COMSOL Multiphysics), the spatial stochastic process model is based on Gaussian Random Fields (R). The model is applied to investigate the degradation behaviour of pesticides in a range of soils through variation of the degree of heterogeneity. This underlines the significance of the effect of soil structure and microbial activity field on transport and degradation of pesticides.

LC01P - Development in life cycle inventory analysis and modelling

MO 098
LCA studies of biofuels in multi-output biorefineries

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The holistic nature of Life Cycle Assessment (LCA) is becoming an indispensable feature in the assessment of sustainable development of society. It is therefore integrated more
and more in decision making, where especially the Carbon Footprint is the exponent of the increasing popularity of LCA. However, several methodological choices still cause discrepancies in the final results, where the allocation procedure is a key issue. Much can be learnt from the current situation, where different regions propose new Carbon Footprint methodologies, with their own specific methodological choices. This causes problems when incorporating LCA results, such as the greenhouse gas (GHG) savings of biofuels, into existing legislation. In this work, a case study is executed in a Belgian multi-output biorefinery producing a mix of food, feed and fuel. Results, calculated with a black box and subprocess approach for economical value, mass, energy and exergy allocation, show discrepancies of up to 59% between the same procedure in subprocess and black box allocation, with a factor 4.1 difference within black box allocation approaches and 1.8 within subprocess allocation. The GHG savings of the biofuel versus the fossil fuel equivalent are up to 80%. When considering a broad waste definition, as is suggested by some methodologies, GHG savings range up to 80%. This work highlights that the subprocess approach is preferred, as this reflects reality better. Furthermore, physical relationships, and especially exergy, are very useful in allocation, as economical values fluctuate in time, and can cause difficulties in finding representative values of intermediate flows in biofineries.

MO 099
A mini-Delphi approach to consensus
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The Delphi method was originally developed as a forecasting method in which a panel of experts is used in a structured manner aiming to a common understanding. We used a version of Delphi to resolve a methodological problem where there is no objectively correct solution: deciding the primary energy factor of industrial waste heat, gas heat generated as byproduct, and heat produced from waste, when these are used for district heating in Sweden. In this context, the aim was not to find acorrect answer but to take advantage of the structured Delphi procedure, including its psychological effects, to reach consensus. Our approach was a mini-Delphi: a one-day workshop with 12 participants representing a variety of stakeholders. After an introduction to the methodological approach and a short questionnaire, the participants discussed the primary energy for the heat source in three groups to improve their understanding of the issue. Each participant then individually put a sticker on a numerical scale to represent the primary energy factor that the participants felt appropriate for the heat source discussed. When all participants did not immediately agree, the participants with the extreme values agreed on the decision. All participants who then allowed to revise their decision. Only one such iteration was made for each heat source due to the time constraints of the workshop. The approach yielded consensus on that waste heat should carry zero, and that heat as a byproduct should carry only primary energy corresponding to the increase in primary energy demand of the industry selling the heat. The workshop also converged on the view that waste that should not be recycled should carry zero or very little primary energy when used as fuel. Similar exercises can be performed to search for consensus in other methodological issues such as allocation of emissions from multifunction processes.

MO 100
The Cereal Unit allocation as a new allocation procedure for agricultural life cycle assessments
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Background

For agricultural life cycle assessments (LCA) several different allocation approaches are currently used. This leads to a broad range of results. In addition, parts of the environment, which are not accounted for in agricultural life cycle assessments (LCA) in different ways, especially in different sectors. For instance, heat produced in bakeries and wheat straw used in biofuel production. The users of the individual co-products (baker and biofuel producer) typically do not know of each other and as a result the allocation methods for their individual LCAs are not aligned to each other. This can lead to the situation that the total environmental burden is inadequately materialized. Material and method

Specific requirements for a suitable allocation method for the agricultural sector are defined, which were used to identify the Cereal Unit (CU) as a promising parameter for an agricultural allocation procedure.

Results and discussion

Currently available allocation methods do not satisfy all requirements for the wide range of agricultural products. Therefore, a new allocation approach based on the Cereal Unit is suggested. The Cereal Unit has been developed since decades for purposes of agricultural statistics and is optimized continuously. It is based on physical, chemical and nutritional factors. The Cereal Unit considers, almost all agricultural products can be allocated based on one common parameter. Exemplary results will be shown, among others, for wheat, rapeseed and sugar beet.

Conclusions and recommendations

The Cereal Unit allocation approach allows using one common allocation procedure within agricultural LCAs by meeting the requirements of this sector. This approach could help to solve allocation problems and might lead to more robust LCA results for services and products originated from agricultural raw materials. We recommend investigating the applicability of the Cereal Unit as allocation approach for agricultural LCAs.

MO 101
Life cycle analysis (LCA) applied to process, integration of process modelling in the building of life cycle inventory - example of a bio-polymer production process
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Life Cycle Assessment (LCA) methodology is a well-established analytical method to quantify environmental impacts, which has been mainly applied to products. However, it also has the potential as an analysis and design tool for processes [1]. One of the interesting identified challenges of LCA applied to processes is the consideration of the operating conditions in the building of Life Cycle Inventory. It allows taking into account processes as complex systems instead of black boxes and considering the environmental impact of the used operating conditions. This could be then interesting in multi-objective optimization (e.g. technical, economic and environmental) of processes and help the stakeholder in decision making process at the time of scale up. This work is based on the case study of an existing pilot process for the production of a biopolymer from wheat straw and bran. An original production process, based on twin-screw extrusion and ultrafiltration processes has been developed. A first cradle-to-gate LCA has been lead in order to help the choise into different options for unit processes and then to identify the hotspots of the process. These data have been modeled and building using Excel flowsheet, and twin-screw extrusion was studied through experimental design. Both of these tools provide inventory data for several operating conditions and have been coupled to LCA with the aim to obtained results about the environmental impacts of each process unit depending on its operating conditions.

This paper gives new perspectives in the fields of LCA applied to process industry: instead of using the methodology as an assessment method coming at the end of the process design, these one is rather integrated at the early stage of process conception with other parameters like economics and technics.

MO 102
Exergy analysis and LCA - a design for environment approach of energy conversion processes
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LCA has been applied widely to design for environment (DfE) of energy conversion processes. It covers the environmental impacts from fuel consumption and the construction, operation, maintenance and disposal of plant components. However, due to the methodological scope of LCA, the environmental impact is related to the product of the energy conversion process, for example to the amount of electric energy generated by a power plant. Especially the functional interdependencies between the process components are not known due to the lack of a harmonized physical base of all modelled plant components.

This gap can be closed by an exergy analysis which enables the allocation of environmental impacts to exergy streams as thermodynamical basis for the overall process. To minimize the impacts environmental impacts of all energy conversion processes, the exergy destruction has to be minimized. A new methodological approach has been developed based on the combination of exergy analysis and LCA. The so called exergoenvironmental analysis assigns environmental impacts to exergy streams. It identifies the environmentally most relevant process components as well as possibilities for the optimization of plant components. As a case study, an energy conversion process consisting of a high temperature solid oxide fuel cell (SoFC) integrated with an althothermal biomass gasification has been analyzed. The investigation reveals the components which have the greatest environmental impacts caused by their thermodynamic inefficiencies and their life cycle (component-related) respectively. It is shown the distinctions between the results of the LCA and the exergoenvironmental analysis, as well as the influence of the exergy destruction on its environmental impacts.

MO 103
Hybrid approaches in life cycle assessment
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With the ultimate goal to assess the greenhouse gas emissions of the livestock supply chain in Italy, different life-cycle based methodologies were reviewed with the aim to apply the most appropriate one. Input-Output Assessment (IOA) and Life Cycle Assessment (LCA) are two of them, which have both been applied for this specific aim. Both these methods have limitations, and the use of both methods has some advantages and limitations. Hybrid methods have the advantage of incorporating the details of a product perspective given by LCA, with the completeness of the economy-wide accounting of IOA. Therefore, theoretically they are considered a promising approach for solving the micro (product) and the macro (economy-wide) level, which is the core of our goal. Several Hybrid methodologies have been proposed, with not always a clear distinction among them. We identified three main categories, namely Tiered Hybrid Analysis (THA) and one other (Olso and others Tuset et al. 2004), Input-Output Hybrid Analysis (IOHA) reviewed by Joshi (2000) and Integrated Hybrid LCA (IHLCA) developed by Suh and Huppes (2005).

IOHA is the most applied followed by THA and IHLCA, in the area of energy, forest, fuel and waste hybrids. Method have been used also for the comparison of different life cycles as organic and conventional farming techniques, and for the environmental assessment of regions and countries. When compared, Hybrid methods often show a higher emission level than LCA or IOA, explaining why they are often considered as a more complete assessment. However, this higher value can also be caused by double counting
Multi-dwelling modeling in LCA - the assessment of household consumption in Swiss communities

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Environmental consumption analyses mostly focus on countries and whole economies, because for this level economic input-output tables are available that allow for environmental extended input-output analysis. However, at the same time, the degree of freedom and type of decisions to be taken in waste management decision making is increased, as well as the availability of data that can be used for LCA, such as shadow prices, ecoinvent databases, and reference product models. The objective of the poster presentation will be to identify a suitable reference system, and to compare the new power plant concept with other power plant concepts, including both dedicated waste treatments and co-processing activities. These models enable the quantification of the direct emissions and the resources consumed as a linear programming (LP) model, comprising two main sets of equations. The first includes mass and energy flow-based process models of common treatment options, including both dedicated waste treatments and co-processing activities. These models enable the quantification of the direct emissions and the resources consumed according to the amount and type of waste to be treated. The second set of equations determines the life cycle inventory (LCI) of inputs and outputs associated with the system operation. The life cycle inventory can be further translated into the associated impact assessment model, and the model output is the optimal allocation of waste and resources to the available or planned waste treatment infrastructure. This allocation should ensure a given required functional unit (FU) of waste treatment and industrial productivity) while conforming to the constraints imposed by the regional context. The capabilities of the approaches presented are illustrated through a case study. Numerical results highlight the importance of considering multiple objectives to avoid shifting burdens between impact categories. In addition, the environmental relevance of shadow prices, i.e., the marginal environmental impact of tight constraints, is discussed as an approach to analyze the uncertainties and benefits for society. The ultimate purpose of our tool is to guide policy makers and practitioners towards the adoption of waste management patterns with improved environmental performance.
On strong and poor arguments for carbon capture and utilization: an LCA perspective

MO 110

Categorizing spatial heterogeneity using GIs: an LCA case study of pressure management in geologic carbon sequestration

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Life cycle stages for emerging environmental impact mitigation technologies require assessments within a real-world context in order to accurately predict economic, environmental, and social impacts in LCAs. Unlike a product in circulation, emerging technologies have yet to interact with markets, environments, laws and cultures. Because of this strongly influencing feature, it is important to understand the importance of economic impacts, and up front, for emerging technologies. In this work, we have investigated and assessed a pressure management technology within the Life Cycle Phase Assessment (LCPA) methodological framework. The LCPA methodological framework allows for the assessment of emerging technologies within the Life Cycle of an emerging technology (LCTEM) is a methodological framework that allows for the assessment of emerging technologies within the Life Cycle of an emerging technology (LCTEM). A pressure management technique reduces the cost of CO2 capture and storage (CCS) by improving the performance of CO2 capture systems. This study evaluates the energetic and environmental benefits of a pressure management technique for CCS using a life cycle assessment (LCA) methodology. The results of this study show that pressure management techniques can reduce the cost of CO2 capture and storage by up to 50%

MO 111

Utilization of CO2 captured in coal power plants for photocatalytic methanol production - ecological implications

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Carbon Capture and Utilization (CCU) is most often motivated using environmental ad-hoc criteria like CO2 balances, fixation amount and fixation duration. In this work, we evaluate the potential of these criteria to drive the development of new technologies. The Life Cycle of an emerging technology (LCTEM) is a methodological framework that allows for the assessment of emerging technologies within the Life Cycle of an emerging technology (LCTEM). This study evaluates the energetic and ecological benefits of the utilization of CO2 captured in coal power plants for photocatalytic methanol production. The results of this study show that the utilization of CO2 captured in coal power plants for photocatalytic methanol production has the potential to reduce the CO2 footprint of methanol production by up to 90%

MO 112

Life cycle risk assessment (LCRA): description of this methodological proposal and a case study

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Life cycle risk assessment (LCRA) is an emerging methodological tool that can be used to evaluate the potential environmental impacts of emerging technologies. The objective of this work is to present an overview of the methodology and to provide a case study to demonstrate its applicability. The results of this study show that LCRA can be used to evaluate the potential environmental impacts of emerging technologies in a systematic and comprehensive manner.

MO 113

Life cycle risk assessment (LCA): description of this methodological proposal and a case study

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Life cycle risk assessment (LCA) is a well-established methodological tool that can be used to evaluate the potential environmental impacts of emerging technologies. The objective of this work is to present an overview of the methodology and to provide a case study to demonstrate its applicability. The results of this study show that LCA can be used to evaluate the potential environmental impacts of emerging technologies in a systematic and comprehensive manner.

MO 114

Adapting life cycle assessment for multi-criteria analysis of a complex system: case study of urban mobility

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Urban mobility is identified as one of the most CO2 emitters in France: transport represents 34% of CO2 emissions in France in 2006 (ADEME 2006), including 25% of urban trip emissions. Some previous studies compare transport modes (Finkbeiner & Al 2006), or assess CO2 emissions that are related to urban mobility on a real case
The first results consist of a complete definition of the system that is based on a segmentation of urban mobility into sub-systems that constitute the “goals and objectives” step in LCA. This decomposition prepares to the next step in LCA, in which modular splits will be aggregated with elementary assessments of modes to obtain a multi-criteria analysis of several scenarios.

The final aim is to provide a configurable method for assessing urban mobility impacts, taking into account societal indicators beyond the environmental ones (such as noise, satisfaction of consumers, time travel, costs etc) will be studied. The final aim is to provide a configurable method for assessing urban mobility impacts, taking into account societal indicators beyond the environmental ones (such as noise, satisfaction of consumers, time travel, costs etc) will be studied.

The ageing and oxidation stability gets increasing importance, since it determines the service life of lubricants in tribological systems in addition to the storage time. With the additional characterisation of conditional-use changes in ecological characteristics allows a comprehensive assessment and is still largely unknown, but an important aspect in terms of LCA for biogenic hydraulic fluids. This methodological approach thus allows the feedback of the desired product properties on the production method.

After tribological application in an ageing test bench (48-192 h) there was only an increasing toxicity for the algae growth inhibition test as a function of time in contrast to the latter being appreciably more difficult to quantify with regard to the consequences of both emissions and accidents. Results of this initial study show not only similar orders of magnitude for impacts related to accidents but that, depending on the perspective applied to the characterisation of emissions-related impact factors and the current trends for both impact types, the impacts of accidents could still be higher.

A comparative life cycle assessment between two different food packaging systems has been carried out: a commercial food packaging film based on polypropylene (PP) and a non-biodegradable and impact heavily on the environment. For all these reasons, a new biodegradable packaging material based on renewable raw materials has been developed. Chitosan is the second most abundant polysaccharide found in nature and has non-toxic biodegradable, and antimicrobial characteristics, which are of great interest for food packaging purposes. Chitosan is mainly manufactured from crustaceans due to the large amount of its skeleton available as a by-product of food processing. It is one of the best available technologies to obtain biofuels from vegetable oil at present. This study presents the GHG emissions of the biofuel HVO (Hydrotreated Vegetable Oil) mixed with mineral diesel. Results highlight that the HVO mixed with mineral diesel has at least the same environmental performance compared to a mixture of FAME and mineral diesel. GHG emissions savings compared to standard diesel from Renewable Energy European Directive 2009/28/Ec are exposed. In addition, sensitivity analysis have been conducted in order to assess the influence in results of different data sources and different allocation processes that LCA standards suggest, showing the most relevant hot-spots that influence the improvement of previous results.

The life cycle inventory for chitosan powder from crustacean shell was taken from literature and film manufacture data was measured directly by our research group in the lab. The EcoIndicator 99 method was selected for comparison and end of life. The data relating to PP packaging films were obtained from Ecoinvent v2.0 database, developed.

Due to the quantification of metal content with ICP-MS in used hydraulic fluids and resultant WSF as well as the determination of the aqueos available metal content, there is a better interpretation and distinction of age-related aquatic ecotoxicity. The additional characterisation of conditional-use changes in ecological characteristics allows a comprehensive assessment and is still largely unknown, but an important aspect in terms of LCA for biogenic hydraulic fluids. This methodological approach thus allows the feedback of the desired product properties on the production method.
acetic acid used in film manufacture and, in a significant way, to the hydrochloric acid used in the raw materials extraction, which is also responsible for the impact in minerals category in the raw materials extraction stage. In addition, the main responsible for the land use is glycine used in the film manufacture considered as a by product from biodiesel.

MO 120
Environmental indicators, as a result of the Life Cycle Assessment application for the Mexican corrugated cardboard industry
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Considering the present situation in Mexico, the environmental protection and the responsible use of the available resources are current needs. The involvement of each of the industries in the country is essential to achieve tangible results for the environmental welfare.

The Life Cycle Assessment (LCA) is used for this study with the objective of making a comparison between the use of virgin, and the use of recycled raw materials in the process of corrugated cardboard, under Mexican conditions. The contribution of applying LCA works to identify different environmental impacts from the individual processes of the complete system.

The identification of the environmental impacts runs in order to consider specific aspects, which would focus on the sustainability of the enterprises involved in the corrugated cardboard manufacturing industry. The aspects identified could be properly implemented in the future as a functional part of an environmental policy proposal.

The results showed that the system of the recycled corrugated cardboard production impacts less in every environmental impact category analyzed, than the virgin corrugated cardboard production. However, in Mexico, it is a system that can be optimized through specific activities; especially in manufacturing and transportation processes, where the greater environmental impacts were located.

MO 121
GHG emissions comparison of tissue paper from virgin pulp vs recycled waste paper
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Pulp and paper manufacturing industry is the fourth largest greenhouse gases (GHG) emitter and is responsible for around 9% of the total global CO2 emissions from manufacturing sectors. The increasing trend of paper consumption is one of the principal drivers behind the emissions from the sector. Therefore, policy measures which ensure not only the reduction in consumption of paper but also the increased use of recycled waste paper, the implementation of cleaner production practices and the use of fibres from sustainable sources are of major importance.

The aim of this work is to compare the environmental implications of tissue paper produced from virgin pulp (VP) vs recycled waste paper (RWP). By doing so, this work informs decision-makers both at company or national levels on the main driving forces behind emissions generation and suggests necessary actions to decrease pollution. The main questions which this work addresses are: how the choice of raw materials for the VP and RWP processes influences the environmental footprint? What are the main drivers behind the emissions? Which are the emission sources? and energy requirements or of transportation? All these aspects are analysed by considering all the stages involved in the life cycle of tissue paper production and identifying the most relevant processes that have significant contribution to the global GHG emissions of the product. Our results show that the energy demand in the form of electricity and steam is relatively higher in the case of RWP process than VP process, if only the manufacturing stages are considered. However, different picture comes out when the comparison is based on the entire life cycle of the product. The GHG emissions from the VP process are about 24% higher than the RWP process. This implies a saving of 424 g eq CO2 for each kg of tissue paper produced from RWP instead from VP. GHG emissions from pulping process alone, 470 g eq CO2 per kg of tissue paper, were about 3 times higher than emissions from waste paper collection and transportation. According to our results, replacing recycled waste paper for virgin pulp has environmental benefits.

EP02P - Endocrine disrupting chemicals: recent developments

MO 122
Combination of Planar Chromatography with in vitro bioassays as a tool for effect directed analysis
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The identification of environmental contamination with a (specific) biological activity is demanding due to the vast number of compounds which are released in the environment by humans. In recent years various strategies and methods were developed for an effect directed analysis which in general combine separation methods like LC or HPLC with biological assays and a subsequent chemical analysis of fractions which are biologically active.

Despite the complexity of chemical mixtures in the environment, the often low concentrations of contaminants are a further challenge, especially in case of anthropogenic micropollutants with specific modes of action like drugs or endocrine disruptors. In order to overcome these difficulties, environmental samples are usually concentrated by solid phase extractions (SPE). However, potential active compounds which are not bound to the matrix of the solid phase are not concentrated and so the SPE might already result in a separation of the sample. They might be even lost if the flow-through of the SPE is not further characterized.

An alternative to the method described above is the use of planar chromatography (HPTLC) in combination with bioassays. Samples can be easily concentrated on a thin layer plate by multiple sample application and/or focusing step if a multi development method is used for the chromatography. The challenge of this strategy is to perform bioassays for the detection of specific effects directly on the surface of the thin layer plate. Therefore, these bioassays have to be adapted for this new application.

The combination of HPTLC with specific bioassays like the Yeast Estrone Screen (YES) is possible. The objective of the presented work is to develop an optimized technique for the combination of HPTLC with various specific bioassays and to test the hypothesis that such an approach is a useful tool for the effect directed analysis of environmental samples.

MO 123
Development of a multi-component detection method for with UPLC-tQ-MS/MS to identify steroid hormones in CALUX positive surface water samples
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Surface waters, such as the rivers Rhine and Meuse, are important sources for the drinking water supply in the Netherlands. Dutch drinking water companies therefore intensively investigate their water sources for the presence of emerging contaminants and their fate during treatment processes. One of the classes of concern are compounds with endocrine disrupting, e.g. estrogenic, activity. Nowadays, natural and synthetic steroidal estrogens are known as the primary causative agents of estrogenic activity in the aquatic environment. With the development of new bioassays, it has become possible to investigate also the activity of other classes of steroid hormones and compounds with comparable or antagonistic activities. Many hormone-like compounds are excreted naturally or are used as pharmaceuticals and might thus enter the environment via similar routes as estrogens. Indeed, using CALUX bioassays for progesteragenic, androgenic, estrogenic and glucocorticoid receptor activation, the presence of especially glucocorticoid activity in Dutch surface waters and glucocorticoids in waste water was recently reported. Now that activity is found, methods are needed for the identification of the responsible compounds.

Due to the low environmental concentrations, an analysis sensitivity is required that is currently only feasible by target analysis methods. We developed a highly sensitive multi-component analysis method for over 40 natural and synthetic steroid hormones in water, including estrogens, androgens, progestagens and glucocorticosteroids. The method uses Ultra Performance Liquid Chromatography separation followed by tandem Mass Spectrometry detection (UPLC-tQ-MS/MS).

We not only had to optimize the first step in the column separation (speed and resolution) but also the second step in the separation: on-column derivatization which is crucial to detect the polar compounds and weak acids. We optimized the first step with the aim to increase the speed and resolution of the separation and at the same time to increase the sensitivity of the detection. For the second step, we investigated a number of on-column derivatization methods. We compared the results with the conventional LC-MS method. The method was applied to samples from Rhine and Meuse and results were compared with results from the CALUX analyses of hormone-like activity in samples from the same sources.

MO 124
Development of simultaneous analysis technique for phthalate di- and mono-esters using online-SPE and high speed mass spectrometer
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Phthalate esters have various homologues with different alkyl side chains. Positive ionisation is more suitable for phthalate analysis. For this kind of analytes, a high speed mass spectrometer is required. Phthalate esters have various homologues with different alkyl side chains. Positive ionisation is more suitable for phthalate analysis. For this kind of analytes, a high speed mass spectrometer is required.

We investigated the application of Ultra High Performance Liquid Chromatography (UHPLC) in combination with solid phase extractions (SPE) for the determination of phthalate esters. The SPE was performed with two different solid phase materials: Oasis HLB and Oasis MAX. Phthalate esters were detected using an ultraperformance liquid chromatography-tandem mass spectrometry system equipped with an on-line solid phase extraction device. The separation of the analytes was achieved by means of a narrow bore (i.d. 2.1 mm) column packed with small C18 particles (size 1,7 μm), improved separation power and detection limits and reduced analysis times are achieved.

The method uses Ultra Performance Liquid Chromatography separation followed by tandem Mass Spectrometry detection (UPLC-tQ-MS/MS). Due to the narrow column, speed and separation power are increased. The separation power is improved without compromising on the separation efficiency. This technique also provides greater reproducibility of pretreatment processes. To achieve high throughput analytical methods, not only the on-line SPE system but also high speed mass spectrometer is required. Phthalate esters have various homologues with different alkyl side chains. Positive ionisation is more suitable for phthalate analysis. For this kind of analytes, a high speed mass spectrometer is required.
Effects of 4-nonylphenol and/or diisononylphthalate on THP-1 cells: impact of endocrine disruptors on human immune system parameters

Hormone Thyroxin (T4), i.e., an aromatic ring with a hydroxyl-group and adjacent halogens. But more recently, also polyfluoroalkyl substances were shown to have moderate enzyme activity of sediment samples from Laguna Lake, Philippines, using the LYES and H295R assays

Compounds that are known to influence the thyroid system (e.g., hydroxylated PBDEs and PCBs, triclosan, DDE, TBBPA) all have structural similarities with the natural thyroid hormones and are capable of interfering with the TH system, an inventory of the literature describing compounds with reported potency to bind to the TH transport protein TTR was made.

In Effect-Directed Analysis (EDA), various bioassays have been implemented that have an endpoint related to endocrine disruption. We have used the radiodissolved TTR-binding assay to detect estrogen activity in sediments from Laguna Lake. In our study, we evaluated the estrogenic activity of the sediment samples by measuring the binding of radioactive TTR to the estrogen receptor in cell cultures. Our results indicate that the sediment samples from Laguna Lake are capable of interfering with the TH system, an inventory of the literature describing compounds with reported potency to bind to the TH transport protein TTR was made. Compounds that are known to influence the thyroid system (e.g., hydroxylated PBDEs and PCBs, triclosan, DDE, TBBPA) all have structural similarities with the natural thyroid hormones and are capable of interfering with the TH system, an inventory of the literature describing compounds with reported potency to bind to the TH transport protein TTR was made.

THP-1 human cell line which was used as a model for macrophages. We used two EDCs, diisononylphthalate (DiP) and 4-n-nonylphenol (NP) alone or in combination in a concentration of 1 µM of combination of NP and DiP induced an IL-8 level in the medium respectively 28.9 and 45% higher than level obtain for control (untreated cells), (ii) to combination

MO 126

Isolation and identification of ligands for the goldfish testicular androgen receptor in chemical recovery condensates from a Canadian bleached kraft pulp and paper mill

The human thyroid hormone system is critical for proper development and function of the body. Any disruption of the thyroid hormone system can have serious health effects. Compounds that interfere with the thyroid hormone system can do so by mimicking the natural thyroid hormones or by blocking their transport to target tissues. Our study aimed to identify such compounds in sediment samples from Laguna Lake, Philippines.

The OH-PBDE congeners most likely originate from human metabolism of the flame retardant polybrominated diphenyl ethers due to the relatively high concentration of PBDEs in the same human blood sample and the strong metabolic relationship between OH-PBDEs and their parent PBDEs.

MO 127

Thyroid hormone disruption in effect-directed analysis - An endpoint of growing concern

Studies of endocrine disruptors have shown that the human immune system is also affected by these compounds. Our study investigated the impact of 4-nonylphenol and diisononylphthalate on THP-1 cells, a human macrophage cell line, to understand the effects of these compounds on the immune system.

MO 128

Estrogenicity of 75 European waste water effluents evaluated by in vitro assay

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Various natural and synthetic contaminants present in urban waste waters have been shown to possess estrogenic activity, and many questions related to the risks of these compounds have yet to be fully understood. Under environmental conditions, steroid hormones appear to be primarily responsible for adverse effects observed in fish downstream of waste water treatment plants (WWTPs). However, instrumental analyses of steroid estrogens often fail in detection of their actual concentrations in complex environmental matrices such as waste water effluents. In the present study, we evaluated estrogenicity of 75 European waste water effluents. The samples originated from SEES 2010 pan-European monitoring campaign coordinated by the European Commission Joint Research Centre (JRC) in Ispra, Italy. Estrogenic activity was expressed as 17β-estradiol equivalents (E2q). Twenty seven sample extracts showed significant estrogenic activity higher than the detection limit 0.5 ng/L E2q with values ranging 0.53 to 17.9 ng/L E2q. The highest activities have been detected in WWTPs at some of the major European capital cities indicating the importance of this study since WWTPs are a major source of estrogenic compounds.

MO 129

Assessing the endocrine disruption of sediment samples from Laguna Lake, Philippines, using the LYEs and H295R assays

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Various natural and synthetic contaminants present in urban waste waters have been shown to possess estrogenic activity, and many questions related to the risks of these compounds have yet to be fully understood. Under environmental conditions, steroid hormones appear to be primarily responsible for adverse effects observed in fish downstream of waste water treatment plants (WWTPs). However, instrumental analyses of steroid estrogens often fail in detection of their actual concentrations in complex environmental matrices such as waste water effluents. In the present study, we evaluated estrogenicity of 75 European waste water effluents. The samples originated from SEES 2010 pan-European monitoring campaign coordinated by the European Commission Joint Research Centre (JRC) in Ispra, Italy. Estrogenic activity was expressed as 17β-estradiol equivalents (E2q). Twenty seven sample extracts showed significant estrogenic activity higher than the detection limit 0.5 ng/L E2q with values ranging 0.53 to 17.9 ng/L E2q. The highest activities have been detected in WWTPs at some of the major European capital cities indicating the importance of this study since WWTPs are a major source of estrogenic compounds.

MO 130

Effect of 4-nonylphenol and/or diisononylphthalate on THP-1 cells: impact of endocrine disruptors on human immune system parameters

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The aim of this study was to investigate the impact of two endocrine disruptors compounds (EDCs) and their human response through a study of their effects on the THP-1 human cell line which was used as a model for macrophages. We used two EDCs, diisononylphthalate (DiP) and 4-n-nonylphenol (NP) alone or in combination in order to evaluate the effects of these compounds on several parameters of the immune response: cytokine secretion, phagocytosis and the putative implication of the estrogen receptors by studying the level of MAPK activation. NP and DiP strongly reduced phagocytosis and modify cytokine secretions. Indeed, THP-1 cell exposures (i) to 5 and 10 µM of combination of NP and DiP induced an IL-8 level in the medium respectively 28.9 and 45% higher than level obtain for control (untreated cells), (ii) to combination
The authors thank the financial support from the Beijing Natural Science Foundation (No. 8101111005060). The University of Hong Kong, Hong Kong, Hong Kong


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SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting

Our results suggest that Medaka primary cell cultures not only serve as a useful tool for screening EDCs but also provide a platform for deciphering the specific target sites of EDCs along the HPG axis and their action mechanisms.
MOL 136

Tetraabromobisphenol-A disrupts thyroid hormone receptor alpha function in vitro: use of fluorescence polarization to assay corepressor and coactivator peptide binding

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Thyroid hormone receptors (TRs) recruit corepressor or coactivator factors to the promoters of target genes to regulate their transcription. Corepressors such as nuclear hormone receptor corepressor (NCoR) are recruited by unliganded TRs, whereas coactivators such as steroid receptor coactivator-1 (SRC-1) are recruited when triggered by the ligand binding domain (LBD). These TRs via a ligand and peptide sequences that can be used to probe the conformational changes induced in TR LBD by TRs. Recombinant LBD of the human TR 1 isoform (TR1 LBD) was produced as a fusion with glutathione S-transferase, and used to develop assays based on fluorescence polarization to quantify the binding of either NCoR or SRC1/2-derived fluorescent peptides to the TR LBD in different conditions. A reciprocal dose-dependent increase in SRC2 peptide binding, in both cases at 50% effective doses. The TR agonists triiodothyroacetic acid and thyroxine were also effective in preventing NCoR peptide binding and increasing SRC2 peptide binding, whereas reverse-triiodothyronine was less efficient and the biologically inactive thyronine had no effect on either process. These experiments were based on the SFA technique, which measured changes in the fluorescence polarization of a fluorescently labeled peptide, as measured by fluorescence polarization, for investigating the conformational changes of TR 1 LBD induced by potentially TR-interfering compounds. Both these methods were used to elucidate the mechanism of the disrupting effects of tetraabromobisphenol-A (TBBPA) on the TR LBD conformation related to the transcriptional activity of the receptor. TBBPA is a flame retardant that is released into the environment, and is a suspected disruptor of thyroid homeostasis. The present results indicate that TBBPA did indeed interfere with the ability of the TR 1 LBD to bind both NCoR and SRC2. TBBPA behaved similarly to T3 in promoting the release of LBD from TR LBD, whereas it failed to promote LBD interactions with SRC2. However, it did reduce the T3-induced interactions between LBD and the coactivator peptide. This study therefore suggests that TBBPA in the micromolar range can affect the regulation of transcription by both the apo- and the holo-TR 1, with potential disruption of the expression of genes that are either up- or down-regulated by T3.

MOL 137

The other endocrine activity in vitro screening of sewage treatment plant effluents for retinoid, thyroid and vitamin D receptor agonists

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In the past, the use of endocrine disrupting chemicals has been paid to environmental chemicals interfering with steroid receptors, especially to estrogenic and androgenic compounds. Doubtlessly, focusing on androgen and estrogen receptors is a plethora of transcription factors controlled by other than steroid hormones. To elude potential effects mediated via non-steroidal hormone receptors to widen the focus to the effects mediated via other hormone receptors.

In this context, we employ Yeast Two Hybrid assays with thyroid receptor (TR), retinoid X receptor (RXR), vitamin D receptor (VDR), and retinoic acid receptor (RAR) to characterize the endocrine activity of 78 effluents sampled at 51 industrial and municipal sewage treatment plants (STP). To avoid the loss of active compounds, wastewater was used for further treatment, e.g. clarification, solid phase extraction (SPE).

STP effluents did not induce TR or VDR activity. Compared to that, 54 of 78 effluents (69%) significantly activated RAR. This activity was very potent, expressed relative to the endogenous ligand all-trans retinoic acid (ATRA), we detected a mean of 241 ng L-1 ATRA-EQ and a maximum of 2160 ng L-1 ATRA-EQ . Since none of the procedures was able to extract significant levels of RAR activity we conclude that the causative chemicals are poorly extractable and thus might be missed when analyzing SPE extracts solely.

In a more general context, our data indicate that the investigated STP are sources of chemicals that activate the retinoic acid receptor. Since the responsible chemicals are so far unidentified, potential in vivo consequences remain to be evaluated. However, in the light of the known teratogenicity of some retinoids, an identification and further toxicological characterization of these ‘emerging’ chemicals is imperative.

MOL 138

The endocrine disrupting effect of hypoxia on pituitary cells

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Hypoxia is an endocrine disruptor which can affect the synthesis and release of sex hormones and thereby impairs reproduction of fish. However, the precise mechanisms of endocrine disruption remain unclear. Moreover, effects of hypoxia on reproduction in higher vertebrates such as mammals remain largely unknown. Gonadotropin releasing hormone (GnRH) is known to play a pivotal role in vertebrate reproduction. Previous studies have suggested that suppressed expression of GnRH and/or GnRH receptor (GnRHR) along the Hypothalamus-Pituitary-Gonad (HPG) axis could be an important mechanism contributing to reproductive impairments in hypoxic fish. Given that the HPG axis and genes controlling steroidalogenesis as well as the sex hormones are highly conserved across vertebrate groups, the endocrine-disrupting effects of hypoxia found in fish also occur in mammals including human. The aim of the present study is to determine whether hypoxia would affect the expression of GnRHR gene (one of the genes of concern) in male and female pituitary cells. A mouse pituitary cell line, LbetaT2, was used in an in vivo model to test the hypothesis that hypoxia could affect the expression of GnRHR in pituitary, thereby affecting reproduction in mammals. LbetaT2 cells were incubated for 24, 36, or 48 hours in a hypoxia chamber with 2% O2 and 98% N2. The cell line was then stimulated with hypothalamic GnRH. The expression of GnRHR increased over time in a hypoxia-dependent manner. The expression of GnRHR was also increased by the addition of testosterone. These data suggest that hypoxia causes the GnRHR expression to be increased in these cells, which may be related to hypoxia-induced changes in the GnRHR expression.

MOL 139

Gamarus palpus responses to short-term exposure towards endocrine disruptors and pharmaceuticals in waste water

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Gamarus palpus is one of the most frequent and abundant freshwater amphipod in European streams, playing an important key-role in the aquatic food web and detritus cycling. Moreover, Gamarus palpus is sensitive towards pollution. Endocrine disruptors and pharmaceuticals are important chemicals in the effluent of urban waste water treatment plants. Studies on the impact of estrogens on aquatic organisms have shown that estrogens can cause changes in the behavior and development of invertebrates. However, the impact of pharmaceuticals on aquatic organisms is still largely unknown. Therefore, the present study aimed to investigate the effects of three pharmaceuticals (BTX, Bti, and Bti2) on the behavior and development of Gamarus palpus. The effects of these pharmaceuticals on the behavior and development of Gamarus palpus were investigated in a chamber experiment. The results showed that BTX and Bti induced a decrease in activity, whereas Bti2 had no effect. In addition, the effects of BTX and Bti on the survival of Gamarus palpus were investigated. The results showed that BTX and Bti induced a decrease in survival, whereas Bti2 had no effect. In conclusion, the present study showed that BTX and Bti have a negative impact on the behavior and development of Gamarus palpus, whereas Bti2 has no effect. However, the effects of all three pharmaceuticals on the survival of Gamarus palpus were not significant.

MOL 140

Do environmental thuringiusiae insectisida products affect the endocrine system?

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Mosquitoes are well known as vectors for many pathogens, such as malaria (Plasmodium falciparum). Global warming and an increasing formation of potential breading sites for mosquitoes are likely to result in an increased incidence of mosquito-borne diseases. Therefore, potent agents that control of mosquitoes are indispensable. However, use of synthetic insecticides - such as DDT - bears the risk of causing serious damage to wildlife. As a consequence, there is need for alternative insecticides that effectively control pests while not impacting the environment. Over the past three decades a protein from Bacillus thuringiensis israelensis has been successfully used as a biological control agent. However, use of pharmaceuticals - such as DDT - will weaken the detection limit, a method to selectively remove the fatty acids is currently under validation.

The aim of this study was to analyze two Bti fermentation products, one of which has been proven to be active in the LYES assay, for additional endocrine potentials including disruption of steriodogenesis. Bti products of concern were extracted at two different temperatures (30 °C / 60 °C) using liquid pressure extraction. Extracts were then analyzed in the H239B steroidogenesis assay, an in vitro screening assay using a human adrenocortical carcinoma cell line. We focused on major hormones of the adrenal gland - such as estradiol, testosterone, androstenedione, progesterone, 17-hydroxyprogesterone and 21-hydroxyprogesterone - using LC-MS/MS and commercial ELISA kits to quantify hormone concentrations. Preliminary results indicate that both products have no significant effects on hormone production. Furthermore, we are currently
Intersex in Scrobicularia plana: transcriptomic analysis reveals new genes involved in endocrine disruption

In order to identify and characterize putative effects of endocrine disrupting chemicals (EDCs) on gonad development and function, we performed a comprehensive analysis of the transcriptome of Scrobicularia plana, a gastropod species that shows clear signs of intersexuality. Our results indicate that several genes involved in sex determination and hormone signaling are upregulated in intersex individuals, suggesting potential new targets for EDCs. Further studies are needed to confirm these findings and to understand the mechanisms underlying the effects of EDCs on sex differentiation.
In fish acute toxicity test, following discontinuous exposure is only partially reversible and may thus have serious implications for fish.

Can fish embryos help predict endocrine disruption? An example with genistein.

MO 147

In this context, we studied the suitability of fish embryos for testing and analyzing endocrine disruption, using genistein as a model substance. Fish embryos are not regarded as protected animals even though their use allows effects to be assessed in a living organism. The drawback of fish embryos is that they are sexually undifferentiated and conventional endocrine disruption assays are biased. Hence, to overcome this obstacle, we used the transcriptomics approach to test endocrine disruption.

We chose two complementing fish species in terms of embryogenesis time and sexual differentiation, zebrafish and medaka. For zebrafish, microarray experiments were conducted, whereas for medaka, gene expression was selected on the basis of screening three genistein genes was assessed by quantitative PCR. Functional gene enrichment analysis of the transcriptional microarray data identified several affected pathways, including pro-apoptotic signaling and the disruption of brain and nervous system development. Hox genes were downregulated. Further, the estrogenic biomarkers aromatase b (cyp19a1b) and vitellogenin (vtg1) were already upregulated at low genistein concentrations (EC10), emphasizing the high oestrogenic potential of genistein. These biomarkers had also been induced in medaka, additionally to species-specific responses, including estrogen receptor 2a gene induction.

In conclusion, the transcriptome response of zebrafish revealed key mechanism of genistein’s molecular action, whereas with the medaka data, a more in-depth insight in the estrogenic mechanisms was achieved, making both fish species complimentary. Overall, we demonstrated that combining fish embryo testing with transcriptomics emerges as a beneficial and animal-free approach for testing endocrine disruption.

MO 148

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MO 149

Beyond designed properties, plant protection products, biocides, pharmaceuticals and other chemicals may pose undesired impacts on aquatic environment via sewage. BP-3 has been detected in surface water, wastewater and in biota. To date, still little is known about the fate and effects of this compound. BP-3 and some of its metabolites, which comprise of benzo[di]thiophene-motie isomers, were previously shown to have estrogenic effects in fish in vitro and in vivo. In our study, effects of BP-3 are evaluated after an exposure of adult male zebrafish (Danio rerio) and zebrafish embryos for 14 days and 120 hours post fertilization, respectively. Exposure concentrations of BP-3 are 10, 200 and 600 µg/L, as confirmed by LC-UV. The water analysis indicates that within 48 hours adult zebrafish, but not embryos, transform BP-3 in part to benzo[di]thiophene-1 (BP-1), an estrogenic compound also used as UV filter. BP-3 and BP-1 are accumulated in fish up to 21 µg/g and 266 ng/g, respectively. We analyse molecular effects by whole-genome transcriptomics (microarrays) and find no significant transcriptional changes. However, 342 transcripts are altered belonging to different pathways. By applying a target gene expression analysis focusing on the estrogenic potential of genistein. These biomarkers had also been induced in medaka, additionally to species-specific responses, including estrogen receptor 2a gene induction.

In conclusion, the transcriptome response of zebrafish revealed key mechanism of genistein’s molecular action, whereas with the medaka data, a more in-depth insight in the estrogenic mechanisms was achieved, making both fish species complimentary. Overall, we demonstrated that combining fish embryo testing with transcriptomics emerges as a beneficial and animal-free approach for testing endocrine disruption.

MO 150

Reversibility of endocrine disruption in zebrafish (Danio rerio) - comparison of different effect levels.

Endocrine Disrupting Chemicals (EDCs) exert effects at very low concentrations and can cause serious problems for the hormonal balance of various organisms. Exposure of wildlife to EDCs is not necessarily continuous, but may often occur in pulses. Consequently for the evaluation of the long-term effects on populations, it is essential to know under which conditions related effects are reversible. Three different substances selected for different modes of action were tested for their long-term impact on sex ratio, gonad development, vitellogenin (VTG) induction and aromatase activity in zebrafish; the androgen trebunel binds directly and very effectively to the aromatase. Ethinylestradiol, a synthetic derivative of estradiol, causes feminization in wildlife and humans. The fungicide prochloraz acts as an aromatase inhibitor by direct interference with the aromatization of androgens to estrogens. All compounds have previously been shown to cause striking effects in zebrafish, but recovery has never been studied in detail or in order to test whether EDC-related effects are reversible, an exposure scenario limited to 60 d was followed by a recovery period of 40 d or continued exposure after 40 d. Four effects levels were examined: (1) population level: sex ratio; (2) organism level: growth; (3) organ/tissue level: histology of gonads (light microscopy); and (4) molecular level: vitellogenin induction (ELISA) and aromatase expression (RTq-PCR).

Results show clear correlation of effects on all levels, but clear-cut differences between the two different exposure groups. We conclude that endocrine disruption in zebrafish following discontinuous exposure is only partially reversible and may thus have serious implications for fish.

MO 151

Testing chemicals for endocrine activity by 21-day fish screening assay.

Bearing in mind that low concentrations of estrogenic compounds can cause severe reproductive problems for the human population, fish and wildlife.

Endocrine Disrupting Chemicals (EDCs) exert effects at very low concentrations and can cause serious problems for the hormonal balance of various organisms. Exposure of wildlife to EDCs is not necessarily continuous, but may often occur in pulses. Consequently for the evaluation of the long-term effects on populations, it is essential to know under which conditions related effects are reversible. Three different substances selected for different modes of action were tested for their long-term impact on sex ratio, gonad development, vitellogenin (VTG) induction and aromatase activity in zebrafish; the androgen trebunel binds directly and very effectively to the aromatase. Ethinylestradiol, a synthetic derivative of estradiol, causes feminization in wildlife and humans. The fungicide prochloraz acts as an aromatase inhibitor by direct interference with the aromatization of androgens to estrogens. All compounds have previously been shown to cause striking effects in zebrafish, but recovery has never been studied in detail or in order to test whether EDC-related effects are reversible, an exposure scenario limited to 60 d was followed by a recovery period of 40 d or continued exposure after 40 d. Four effects levels were examined: (1) population level: sex ratio; (2) organism level: growth; (3) organ/tissue level: histology of gonads (light microscopy); and (4) molecular level: vitellogenin induction (ELISA) and aromatase expression (RTq-PCR).

Results show clear correlation of effects on all levels, but clear-cut differences between the two different exposure groups. We conclude that endocrine disruption in zebrafish following discontinuous exposure is only partially reversible and may thus have serious implications for fish.

MO 152

A comprehensive study on the toxicity of triphenyltin chloride to the rotifer Brachionus sp. at different biological organisation levels.

A detailed study on the toxicity of triphenyltin chloride (TPTC) to the rotifer Brachionus sp. was conducted, where toxicological effects of TPTC were assessed by different endpoints. The water analysis indicates that within 48 hours adult zebrafish, but not embryos, transform BP-3 in part to benzo[di]thiophene-1 (BP-1), an estrogenic compound also used as UV filter. BP-3 and BP-1 are accumulated in fish up to 21 µg/g and 266 ng/g, respectively. We analyse molecular effects by whole-genome transcriptomics (microarrays) and find no significant transcriptional changes. However, 342 transcripts are altered belonging to different pathways. By applying a target gene expression analysis focusing on the estrogenic potential of genistein. These biomarkers had also been induced in medaka, additionally to species-specific responses, including estrogen receptor 2a gene induction.

In conclusion, the transcriptome response of zebrafish revealed key mechanism of genistein’s molecular action, whereas with the medaka data, a more in-depth insight in the estrogenic mechanisms was achieved, making both fish species complimentary. Overall, we demonstrated that combining fish embryo testing with transcriptomics emerges as a beneficial and animal-free approach for testing endocrine disruption.

MO 153

A comprehensive study on the toxicity of triphenyltin chloride to the rotifer Brachionus sp. at different biological organisation levels.
Sexual endocrine disruption in fish with focus on estrogen receptor antagonists- a fish life cycle test with fulvestrant

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MO 157

Sexual endocrine disruption in fish with focus on estrogen receptor antagonists- a fish life cycle test with fulvestrant

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MO 153

Expression of all-trans and 9-cis retinoic acid receptor (RAR/RXR) genes during the zebrafish early development

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External endocrine disruptors have been shown to interfere with the development of the sex organs of fish (genitalia and gonads) during the first 24-48 hpf (hours post fertilization), as well as with the development of gonadal function in the adult stage. The zebrafish genome encompasses no less than 10 different genes coding either for retinoic acid (RAR) or 9-cis retinoic acid (RXR) receptors, which participate in the transcriptional activity of these genes. Induction of steroidogenic genes could be interpreted as a compensatory biological response to inhibition of cytochrome P-450 dependent steroidogenic enzymes. In vitro testicular explants were exposed to similar concentrations of clotrimazole, and no effect was observed on transcript levels of the 11-KT synthesis genes. The zebrafish genome encompasses no less than 10 different genes coding either for retinoic acid (RAR) or 9-cis retinoic acid (RXR) receptors, which participate in the transcriptional activity of these genes. Induction of steroidogenic genes could be interpreted as a compensatory biological response to inhibition of cytochrome P-450 dependent steroidogenic enzymes. In vitro testicular explants were exposed to similar concentrations of clotrimazole, and no effect was observed on transcript levels of the 11-KT synthesis genes.
MO 158
Sub-lethal effects of mixture of compounds in Zebrafish (Danio rerio)

Sub-lethal effects of mixture of compounds in Zebrafish (Danio rerio) was assessed. In this study, we evaluated estrogenic activity of ten BPs in a model fish species, the zebrafish (Danio rerio), by combining newly developed in vitro and in vivo models. In vitro, three specific zebrafish reporter gene models expressing zebrafish estrogen receptors (ZiERs) in zebrafish hepatic cell line (ZFL) were used. Estrogenic activity of BPs was quantified by in vivo using a newly developed transgenic zebrafish line that expresses GFP under the control of the estrogen receptor alpha (ERα) promoter. The expression of GFP was used as an endpoint to assess the estrogenic activity of BPs. Overall, the results showed that some BPs, such as THB, BP1, 4BP, while BP and 234 BP were non-active. We noted differences in BPs ranking depending on the reporter gene used to detect estrogenic activity.

MO 159
Zebrafish embryos as bioassay tools for detection of estrogenic and dioxin-like chemicals in environmental matrices

Benzophenone derivatives (BPs) are used as UV filters in many different products. In this study, we evaluated estrogenic activity of ten BPs in model fish species, the zebrafish (Danio rerio). We used a newly developed transgenic zebrafish line expressing green fluorescent protein reporter gene under the control of estrogen receptor alpha (ERα) promoter. The expression of GFP was used as an endpoint to assess the estrogenic activity of BPs. Overall, the results showed that some BPs, such as THB, BP1, 4BP, while BP and 234 BP were non-active. We noted differences in BPs ranking depending on the reporter gene used to detect estrogenic activity.

MO 160
Evaluation of estrogenic activities of benzoic derivatives using innovative in vitro and in vivo zebrafish models

Benzophenone derivatives (BPs) are UV filters in many different products. In this study, we evaluated estrogenic activity of ten BPs in model fish species, the zebrafish (Danio rerio). We used a newly developed transgenic zebrafish line expressing green fluorescent protein reporter gene under the control of estrogen receptor alpha (ERα) promoter. The expression of GFP was used as an endpoint to assess the estrogenic activity of BPs. Overall, the results showed that some BPs, such as THB, BP1, 4BP, while BP and 234 BP were non-active. We noted differences in BPs ranking depending on the reporter gene used to detect estrogenic activity.

MO 161
Endocrine disrupting effects of OSPW and ozonated OSPW on sex steroid synthesis and signalling in fathead minnows

OSPW has endocrine disrupting effects on exposed fish and in vitro. Although ozonation attenuates some of the endocrine disrupting effects of OSPW the effects of ozone-treated OSPW on sex-steroid production and signaling in fish is unknown. In this study, sexually maturing male and female fathead minnows were exposed to either control freshwater, OSPW or ozonated OSPW to demonstrate the endocrine disrupting effects of OSPW. The abundances of transcripts of estrogen responsive genes were quantified by quantitative real-time PCR (qPCR) in male and female fathead minnows. The results showed that OSPW and ozonated OSPW had endocrine disrupting effects on exposed fish and in vitro. Although ozonation attenuates some of the endocrine disrupting effects of OSPW the effects of ozone-treated OSPW on sex-steroid production and signaling in fish is unknown. 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Head kidney lymphocytes are mainly B-cells, the obtained results strengthen the observation of phagocyting B-lymphocytes in teleosts. The impairment of phagocytosis by estradiol impairs head kidney leukocyte phagocytosis in juvenile sea bass (D. labrax L.). The subsequent study. This research is funded by INTERREG IV A (DIESE, #4040) of the European Union. The thymus, were prepared for histological observations in order to assess thymus volume, region volumes and the ratio between cortex and medulla. No differences in thymus concentration of sex hormones in the organism development of the relevant immune organs may be impaired in larvae and juveniles. Sea bass, at different developmental stages of the immune system (30 dph, 90 dph, 120 dph), were exposed to 20 ng/L E2 for 35 days. Phagocytosis of head kidney lymphocytes is one of the rare, established biomarkers for the immune system in ecotoxicology. Intracellular investigation of the thymus immune system, the thymus is in addition to the head kidney considered to be a primary immune organ. It consists of two different compartments: the cortex and medulla. Immature T-lymphocytes migrate from the cortex into the medullary region during their maturation prod lifetime. The critical period in thymic regionalisation lies between 51 and 92 dph in sea bass. The thymus gland is considered to reach adult volume 365 dph. The thymus is particularly susceptible to waterborne pollutants as only an epithelial layer separates it from the gill chamber. In mice it is evident that 17-β estradiol (E2) plays an important role in T-cell maturation, more precisely on the initiation of apoptosis in auto-reactive T-lymphocyte precursors, which occurs at the border between the two thymus regions. As a result of livestock breeding and anthropogenic wastewaters, higher concentrations of oestrogens are present in the aquatic environment, therefore the current study aimed to elucidate the possible impairments of E2, as a model oestrogen, on fish thymus. Juvenile medaka (Oryzias latipes) were exposed to different concentrations of E2 (0; 2; 20; 200 ng/L) for 56 days. The head sections, including the thymus, were prepared for histological investigations in order to assess thymus volume, region volumes and the ratio between cortex and medulla. No differences in thymus volume or regionalisation between (200 ng/L) and control fish could be observed. Nevertheless, E2 might affect the thymus at a sub-cellular level with consequences for thymocyte maturation. For instance, we have shown that the expression of different classes of differentiation (CD)-receptors associated with T-cell maturation in the following study. This research is funded by INTERREG IV A (DISE, #4040) of the European Union. The effects of towel eluates on Vitellogenin levels and EROD activities in rainbow trout (Oncorhynchus mykiss). Effects of 17-β estradiol on thymus volume and regionalisation in juvenile sea bass (D. labrax L.) Reproductively-active male and female fish were exposed to DE-71 (0 [control], 0.65, 1.3, 2.5, and 5.0 μg/L) via flow-through exposure for 21-d and evaluated for survival, reproductive behavior, and secondary sexual characteristics. Reproductive fecundity and fertilization success were monitored daily. At termination, the status of the reproductive organ index was assessed by the gonad-somatic index (GSI), gonadal histology, plasma steroids (estradiol [E2] and testosterone [T]), and 11-ketotestosterone (11-KT). Effects of towel eluates on Vitellogenin levels and EROD activities in rainbow trout (Oncorhynchus mykiss). Effects of towel eluates on Vitellogenin levels and EROD activities in rainbow trout (Oncorhynchus mykiss). Effects of towel eluates on Vitellogenin levels and EROD activities in rainbow trout (Oncorhynchus mykiss).
MO 168

A non-invasive method based on head morphology to sex mature three-spined Stickleback (Gasterosteus aculeatus) in rearing conditions

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The three-spined stickleback (Gasterosteus aculeatus) is a small-bodied teleost fish which is a major component of shallow water food webs in the northern hemisphere. G. aculeatus is a reference species for experimental studies, in particular for the assessment of endocrine disruptors. Sex ratio can bias the outcomes of an experimental study, especially if this study focuses on reproduction or behaviour. Moreover, sex-ratio, by itself, can be a very relevant endpoint in experimental tests. A mathematical model to distinguish mature female and male three-spined Sticklebacks G. aculeatus is proposed. This method is based on sexual dimorphism in the head morphology.

The discrimination was established on five distances of interest on the head, divided by the standard length of fish. The parameters were estimated based on a training set composed of a random character distribution that was statistically validated on a test set composed of 69 fish. Our model permits to balance between the percentage of fish that can be sexed and the percentage of fish correctly sexed. Compared to other available methods to sex G. aculeatus, our model is non-invasive, not expensive, rapid, and reliable, can be calibrated out of the breeding period.

MO 169

Effects of produced water from an offshore oil-platform; an in vivo study using the three-spined stickleback (Gasterosteus aculeatus) as a model species

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There is growing concern over the high levels of anthropogenic pollutants entering the Arctic region. In light of the anticipated expansion of oil exploration and production in Arctic areas, of particular concern is the potential impact of hydrocarbon-related contaminants on the Arctic ecosystems. Several of these compounds are known to exhibit endocrine disrupting properties. The predicted expansion of oil production into Arctic areas would pose a considerable environmental risk, and highlights the need for the implementation of robust indicator species for future biomonitoring programmes.

The three-spined stickleback (Gasterosteus aculeatus) is a small teleost fish widely distributed throughout the Northern hemisphere, occurring as far north as Svalbard. This ubiquitous species is increasingly being recognized as an emerging model in ecotoxicology, notably as a sentinel for endocrine disruption. The stickleback can be used as a combined biomarker of both estrogenic and (anti-)androgenic compounds, and with the sequencing of its genome an increasing number of molecular tools are being developed for the assessment of contaminant exposure. The stickleback has the potential of becoming a valuable indicator species to identify and monitor the impact of anthropogenic pollutants in Arctic ecosystem, and be included in future biomonitoring programmes.

The objective of this study was to evaluate the effects on stress tolerance in fish after exposure to produced water, using the three-spined stickleback as a model organism. Effects were assessed by quantification of gene expressions (UDP-GC, CYP1A, VGT, PLA), in addition to measuring the levels of glucose and cortisol.

MO 170

Bioaccumulation and sublethal toxicity of 4-nonylphenol in chironomus riparius meigen 1804 (Diptera, chironomidae) larvae: assessment of mentum shape variations by means of morphometric analysis

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Bioaccumulation and sublethal toxicity of 4-nonylphenol (NP) was studied in the midge C. riparius. The biomarker used for the assessment of contaminant exposure was the mentum shape variation (MSV). As a combined biomarker of both estrogenic and (anti-)androgenic compounds, and with the sequencing of its genome an increasing number of molecular tools are being developed for the assessment of contaminant exposure. The stickleback has the potential of becoming a valuable indicator species to identify and monitor the impact of anthropogenic pollutants in Arctic ecosystem, and be included in future biomonitoring programmes.

Differentiation and development of gonad did not precede the development of genitalia in the ivory shell, suggesting that regulatory mechanism of reproduction might be different from that of other fish species. Yolk protein levels in different bivalve tissues were determined both by ALP and the developed ELISA and a comparison of results obtained from both methods were made. In addition, river water mussels (Unio tumidus) were exposed to E2 (57, 164 and 512 ng/l) for seven weeks during the reproductive period to investigate if emergence could be induced. Histological examination of the gonads revealed that emergence could not be induced at these E2 concentrations and the presence and quantity of yolk protein in tissue and hemolymph was investigated.

MO 171

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MO 172

Yolk proteins as biomarker for endocrine disruptors in bivalve molluscs


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Endocrine disrupting compounds (EDCs) are known to cause intersex and altered sex ratios in fish but effects of endocrine disruptors on bivalve molluscs have only been reported from a few studies. Yolk proteins in fish are oogenesis-specific proteins, induced during oogenesis, and are downregulated during卵黄 developmental stages in teleosts.

In this work, we studied bioavailability, bioaccumulation and sublethal toxicity of 4-NP by exposing first to four instar chironomid larvae (Chironomus riparius) to a 4-NP concentration of 6.71 and 184.6 mg/kg d. weight; 4-NP in pore-water was monitored for 4-NP, and 4-NP in pore-water was monitored for 4-NP. After 2 days exposure, larvae were removed and 4-NP concentrations in chironomids were determined. In the head capsule, sex ratios were assessed by observing and comparing four sex-specific profiles: (1) the fluctuating asymmetry index via traditional morphometrics; (2) three fluctuating asymmetry indices via traditional morphometrics; (3) this finding fluctuating asymmetry via geometric morphometric analysis; and (4) shape variations between the control group and exposed groups. Bioaccumulation test revealed that the 4-NP uptake in organisms increased with increasing 4-NP concentration in pore water. Nevertheless no correlation could be drawn with either deformities or both factors. Significant shape variation, corresponding to lateral tooth size increases, were detected at 184.6 mg/kg d. weight.

MO 173

Comparison of var sexus and penis development between the rock shell, Thais clavigera (Muricidae) and the ivory shell, Babylonina japonica (Buccinidae)

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The characteristics of the development of male genitalia (penis and var sexus) in imposex-exhibiting female and male rock shells, Thais clavigera (Muricidae), were histologically examined from specimens from wild populations and laboratory-reared females. Penis and var sexus development was already observed in both imposex-exhibiting female and male rock shells even at approximately 6 months old. A variety of var sexus morphogenesis patterns were observed in wild female T. clavigera. The characteristics of var sexus development were summarised. The immature var sexus at an initial stage, however, was only observed beneath or behind the penis, whereas the var sexus at an initial stage was observed close to the genital papula in TBT-exposed females, which was different from the characteristics of var sexus development observed in wild males. Taking into consideration both the observed results from wild female specimens and from TBT-exposed females in the laboratory, the var sexus sequence (VDS) index for T. clavigera was proposed as VDS 1-6. Meanwhile, we also histologically examined development of genitalia in the ivory shell, Babylonina japonica (Buccinidae), using 2-year-old shells from wild populations and laboratory-reared juveniles for 0-20 months of age. Differentiation of gonad (i.e., ovary) was observed before 16 months of age, which was unclear before 16 months of age. The var sexus was observed in males at 14 months of age, although no penis was observed in them. Formed penis was recognized in almost all males at 16 months of age, although var sexus was not yet completely formed. Vagina, bursa copulatrix and capsule gland were developing in 14-month-old females. Albumen gland and receptaculum seminis were also developing in 16-month-old females. Differentiation of posterior genitalia did not proceed to an agent of development of genitalia in the ivory shell, suggesting that regulatory mechanism of reproduction might be different between molluscs (prosobranch gastropods) and vertebrates. Moreover, there might be a considerable degree of difference on var sexus and penis development
between the rock shell, T. clavigera (Mureciidae) and the ivory shell, B. japonica (Buccinidae), namely, even among prosobranch gastropod species.

MO 174

**Impact of Roundup® and 17α-Ethinylestradiol exposure on the liver morphology of bullfrog's tadpoles** (Lithobates catesbeianus)

C. Abdulla1, E.C.M. Silva-Zacarín1

UFSCar, Sorocaba, Brazil

The new European Union Plant Protection Products Regulation (PPPR 1107/2009) identifies the need to consider whether a substance is a potential endocrine disrupter in aquatic non-target organisms and the current draft of the PPP requirements request to screen three assays for ecotoxicological endocrine-disrupting potential. Of these, we describe here our experience in the establishment and validation of the amphibian metamorphosis assay for potential endocrine disrupting chemicals with *Xenopus laevis*.

**Progestins - potent endocrine disrupters of the female reproductive system**

A. Safor, Uppsala university, Uppsala, Sweden

Progestron signalising has received very little attention as a potential target for disruption although it is a key regulatory pathway in the development and function of the female reproductive system. Recent research has shown that exposure to progestins is frequently encountered in the environment of wild fish. Progestins are extensively used in contraceptives and in other hormonal therapies in human and veterinary medicine. More information on the targets and effects of progestins in adult and early life stages is needed to assess the environmental risks of this type of compounds. The main objective of this study was to determine developmental and reproductive toxicity of progestins on the aquatic organism *Xenopus laevis*.

MO 176

**Validation of the amphibian metamorphosis assay for potential endocrine disrupting chemicals with Xenopus laevis**

C.A. Jenkins, J.J. Burlingham, J.B. Pawsey, I. Taylor

Huntingdon Life Sciences, Suffolk, United Kingdom

*A* recent European Union Plant Protection Products Regulation (PPPR 1107/2009) identifies the need to consider whether a substance is a potential endocrine disrupter in aquatic non-target organisms and the current draft of the PPP requirements request to screen three assays for ecotoxicological endocrine-disrupting potential. Of these, we describe here our experience in the establishment and validation of the amphibian metamorphosis assay with *X. laevis* with the African Clawed Frog.

**Progestins: putative endocrine disrupters of the female reproductive system**

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Progestron signalising has received very little attention as a potential target for disruption although it is a key regulatory pathway in the development and function of the female reproductive system. Recent research has shown that exposure to progestins is frequently encountered in the environment of wild fish. Progestins are extensively used in contraceptives and in other hormonal therapies in human and veterinary medicine. More information on the targets and effects of progestins in adult and early life stages is needed to assess the environmental risks of this type of compounds. The main objective of this study was to determine developmental and reproductive toxicity of progestins on the aquatic organism *Xenopus laevis*.

MO 177

**Bioactivation of PBDE-47 by human liver microsomes and Cytochrome P450s and formation of potentially toxic metabolites**

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During the past decade both animal and human studies have supported an association between polybrominated diphenyl ether (PBDE) flame retardants and neurodevelopmental disorders, particularly following in utero and postnatal exposure. Evidence is also growing suggesting that bioactivation by oxidative metabolism adds considerably to the neurotoxic potential of PBDEs. Thus, there is a critical need to further our understanding of PBDE metabolism in humans. This study conducted a qualitative and quantitative characterization of the in vitro metabolism of 2,2',4',4-tetrabromodiphenyl ether (BDE-47), the most abundant congener retained in humans, using recombinant human liver microsomes (0.1 to 10 µM BDE-47). Of the 11 human CYPs that were screened, CYP2B6 was the predominant CYP capable of forming different mono-hydroxylated-BDEs (OH-BDEs), s, including 3-OH-BDE-47, 5-OH-BDE-47, 6-OH-BDE-47, 2'-OH-BDE-66, 4'-OH-BDE-49, and 4'-OH-BDE-49. With the exception of 2'-OH-BDE-66, all of these metabolites have also been detected in human blood samples, supporting the similar in vivo bioactivation of BDE-47. Moreover, the analyses by full scan GC/MS of the metabolites of BDE-47 formed by CYP2B6 showed the formation of di-OH-BDE-47 and di-OH-dioxin, a novel metabolite. Kinetic studies of BDE-47 metabolism by CYP2B6 and pooled human liver microsomes found Km values ranging from 1-2 µM, indicating the high affinity of CYP2B6 for the formation of hydroxylated metabolites. The prominent role of CYP2B6 in the metabolism of BDE-47 will help us better understand how xenobiotics are handled and whether future mechanistic and epidemiological studies investigating the potential of BDE-47 and its’ metabolites to produce neurobehavioral/ neurodevelopmental disorders.

MO 178

**Affect of EDCs on fish communities in the Levuwhu River, Limpopo Province, South Africa**

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Contaminants present within aquatic ecosystems worldwide are the result of agricultural applications, urban development and industrial effluents. Current contamination by DDT in the Limpopo River, Limpopo Province, South Africa is primarily due to IRS (indoor residual spraying) insecticide use to control insect-borne diseases. DDT and its resulting metabolites DDE and DDD may continue to persist in various environmental phases, long after spraying. The characteristically high lipophilicity, chemical stability and low biodegradability render it a high uptake or bioaccumulation. Despite DDT spraying for many years, limited data on these contaminations in aquatic ecosystems are still scarce. We approached human impacts on aquatic ecosystems e.g. water quality, habitat effects or the overall effects on the organism health. A study was therefore done to assess the effect of DDT, its metabolites and other pollutants in the water, sediment and biota in the aquatic ecosystem of the Levuwhu River catchment.

Valuable information on chemical variables were measured to determine water and sediment quality, Available historical water quality data were obtained. Pesticides extracted from water, sediment, and fish tissue were quantified on a gas chromatography mass spectrophotometer (GC-MS). Electron microscopy and seine nets were used for fish sampling from different river habitats. River flow data, occurrence and relative abundance of fish, and non-parametric diversity indices were determined. Relative abundance for fish communities were described employing two statistical models. Selected biomarkers were used to determine sub-cellular effects of EDCs in field sampled fish.

Eutrophication occurs for irrigation, water forestation, community development and extensive rural activities in the in-stream and riparian habitat. These activities yielded impacts such as bank erosion, flow modification, water quality changes, bed modification and some solid waste disposal. Pesticide levels were only above existing guidelines at specific sampling sites. Biomarkers showed effects of the contaminants on sub-cellular to organ levels with no effects on organism survival. No changes in fish community structures occurred while exposed to DDT and other contaminants measured in the streams. The exposure duration and/or concentrations of pollutants were probably too low to induce any effects. Ecosystem services are therefore not negatively impacted.
Distribution of endocrine disrupting pollutants in the Long Island Sound

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Water waste treatment facilities (WWTFs) input fresh water, nutrients, and contaminants to the Long Island Sound (LIS). While nutrient loads and concentrations for some contaminants are known, there are many unknowns about the full range of toxic effects are still to be determined, and the regulatory framework controlling their use and allowable inputs into coastal waters has yet to be established. The water and sediment of the LIS are routinely sampled for concentration data of classical persistent organic pollutants, however there are numerous emerging contaminants, with known endocrine disrupting and bioaccumulating properties, that have yet to be detected in this economically important region. It is critical important to investigate the inputs of emerging contaminant throughout the LIS, in order to determine the potential impacts on this estuarine ecosystem. Eight water waste treatment facilities (WWTF) which discharge directly into the LIS were tested for several classes of known endocrine disrupting compounds (EDCs); perfluorinated compounds (PFCs), phthalates esters (PBAEs), functional compounds (nonylphenol, octylphenol, bisphenol A), and the steroids estrones and estradiol. WWTFs have been shown to be the sources of these compounds, yet partitioning of these compounds is limited.

WWTFs are a known point source of these compounds; research indicates that biodegradation during secondary treatment can increase concentrations of PFCs in wastewater effluent. The distribution of several of the target compounds between the suspended particulate and dissolved phases in the effluent waters was determined to be a function of their molecular weight. This information on environmental occurrence and relevant gene expression analysis in an in-situ study based on environmental occurrence and relevant gene expression analysis in roach (Rutilus rutilus) steroidogenesis: an in-situ study based on environmental occurrence and relevant gene expression analysis in roach (Rutilus rutilus) steroidogenesis: an in-situ study based on environmental occurrence and relevant gene expression analysis in roach (Rutilus rutilus).

Effects of antiandrogenic compounds on roach (Rutilus rutilus) steroidogenesis: an in-situ study based on environmental occurrence and relevant gene expression analysis in roach (Rutilus rutilus). The results show widespread occurrence of target compounds, although the level of concentrations of different compounds detected varied considerably depending on the location and season.

In order to estimate the estrogenicity of samples, the EEQ were calculated using relative estrogenic potency (relative to $17\beta$-estradiol) . As it was expected, the results showed that, especially estradiol, were the largest contributors to the estrogenic potential with values between nd-4.60 ng/L. However the contribution of other compounds such as alkylphenols, BPA and antioestrogens to the total estrogenicity was low and ranged between nd-0.09 ng/L.

Distribution of androgen receptor antagonists in sediments and antiandrogenic effects on gonadal maturation and histology of roach (Rutilus rutilus) collected from three coastal watersheds in the Mediterranean Sea is investigated. Antiandrogenic activity was assessed using the Ovotestis Severity Index (OSI, a novel method) in this study. The estuaries presenting higher rate of OSI, correspond to the higher pollution levels, and show also higher rate of gonad lesions. These data are in correspondence with our published chemical data, as both Mondego and Douro have estrogens in the water (with a lesser load in Mondego). They corroborate that androgenic are waterborne exposed to estrogenic compounds and OSI should be used in this kind of studies.

Supported by FCT project PTDC/MAR/70436/2006 and PhD Grant SFRH/BPD/25746/2005.

Assessment of interspecies variability in grey mullets from three Portuguese estuaries - preliminary data

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All over the world, plentiful chemicals reach continuously the environment, and some of them are endocrine disrupters compounds (CDEs) which can cause diverse harmful effects in wild fish (also under low concentrations) including interspecies variability, namely otovestis (ovocytes in the testis), but can also affect human health. The presence of interspecies in ichthyofauna has been reported in numerous countries, including (scarce information) in Portugal, but no data was published on large sampling and covering several estuaries, and usually no ranking system for severity assessment is done. For this aim, we have been studying adult grey mullets (Mugil cephalus) caught in the estuaries of the rivers Mondego (2006), Douro (2007) and Ave (2008). Collections took place twice a year, aiming 50 animals per survey, in spring/summer (SS) and autumn/winter (AW). So far, the Ovotestis Severity Index (OSI) showed interspecies variability in grey mullets, with SS vs AW: 12 % vs 8 % in Mondego; 30 % vs 8 % in Douro, and 13 % vs 39 % in Ave. Despite the presence of otovestis in all estuaries, the density and oocyte development stage in testis varies greatly.

We used the Ovotestis Severity Index (OSI) in this work (proposed by Bateman et al. 2004). OSI data obtain are (SS vs AW): 0,6 and 0,3 in Mondego mullets, 6,1 and 2,8 in Douro in SS and AW mullets. The OSI was low in Mondego fish, which agree with the 0,8 in unamended estuary studied (our reference estuary). In Douro, the fish present higher OSI, but Ave mullet show the highest value. No seasonal differences were detected in OSI values.

In some cases we observed also considerably differences in histopathology of the gonads (fibrosis, melanomacrophage centers, interstitial inflammation, as well as unspecified inflammation) that can be related to the high pollution levels, and show also higher rate of gonad lesions. These data are in correspondence with our published chemical data, as both Mondego and Douro have estrogens in the water (with a lesser load in Mondego). This work corroborate that mullet are waterborne exposed to estrogenic compounds and OSI should be used in this kind of studies.

Supported by FCT, project PTDC/MAR/70436/2006 and PhD Grant SFRH/BPD/25746/2005.

Assessment of antiandrogenic compounds on roach (Rutilus rutilus) steroidogenesis: an in-situ study based on environmental occurrence and relevant gene expression analysis in roach (Rutilus rutilus).

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Wildlife is exposed to an increasing pollution pressure which can disrupt homeostasis and ultimately fitness of the more sensitive species and may thus lead to biodiversity erosion. For more than a decade, efforts were made by the scientific community, to assess and understand the impact of endocrine disruptors, especially estrogenic compounds, on fish. Feminization and masculinization of fish were demonstrated in the field and correlated not only to estrogenic contaminants but also to antiandogenic compounds. Although less characterized, these latter might be of importance. They can interfere with the androgen pathways at the receptor level and/or by modulating transcriptional or enzymatic activities related to steroidogenesis. In this study, Roach was chosen with regard to its large repartition in freshwater systems and to its sensitivity to endocrine disruption. Four different sites of the Seine river catchment basin in the Seine presenting an overall contamination gradient were studied. Sex and fish bile were sampled in order to determine the occurrence of androgen antagonists in the environment and in the exposed animals using the anti-yeast androgen assay (anti-YAS) assay. Liver and gonad of sexually mature individuals were dissected to carry out transcriptional analysis of key genes involved in steroidogenesis. This includes genes encoding for the steroidal acute antiestrogen protein (SaAR) responsible of the import of cholesterol in mitochondria that represents the rate limiting step of sterol-14 α-hydroxylation, and usually involved in aromatization. The CYP 1A1A (1C22r30c3) and the 1A2 (CYP1A2) genes, which catalyze oxidation and clearance of intermediary steroids; the CYP 1A2, so-called aromatase that converts testosterone in estradiol 17β. Furthermore, transcriptional level of a CYP3A isoform catalyzing sexual steroid maturatization was assessed in order to appreciate whether environmental pollutants disrupt the biotransformation balance of endogenous steroids. To our knowledge, this is the first in situ study that underlines in the same time the occurrence of androgen receptor antagonists in sediments and antiandrogenic effects on gonadal mRNA levels.

Analysis and occurrence of endocrine disrupters and related compounds in surface waters and sediments in rivers of the Iberian Peninsula

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The Mediterranean basin is one of the most vulnerable regions of the world to the global change due their climatic conditions characterized by summer drought and their high coastal and human population density. Moreover, the high activity close to the Mediterranean rivers and the high population density in these areas, are the principals arguments to evaluate the water quality of these rivers.

The objective of this work was the determination of endocrine disrupters and related compounds belonging to different groups of chemical substances (10 estrogens, natural and synthetic, in free and conjugated form, 8 alkylphenols, 4 antiseptics, 2 antibacterials, 3 flame retardants, 2 anticorrosives and BPA) in four representative watersheds in Spain: Llobregat, Ebro, Júcar, and Guadalquivir.

In this study, a multiresidue analytical method for the analysis of water samples was applied, using the Thermo Scientific Equan LC-MS system, an automated online preconcentration system (PEL) was carried out using a fully automated ASE 200 system (Dionex, Sunnyvale, CA, USA), the solvent extraction was methanolaceton (1:1) mixture, for clean-up a solid phase extraction (SPE) was performed. A Thermo Scientific TSQ Vantage triple quadruple mass spectrometer with an ESI source was used for the MS analysis. The objective of this study was to determine occurrence and concentrations of different compounds detected varied considerably depending on the sampling point. For example, in the case of water samples the 3 compounds with higher contribution in terms of concentrations were alkylphenolic, corrosives and phosphonorous fatty acid derivatives with levels between nd-10 to pg/L. The natural and synthetic estrogens in free and conjugated form were found in some points in levels lower than 1 pg/L.
Alkylphenolic substances and BP

Determining outliers in fathead minnow (Pimephales promelas) plasma vitellogenin concentration and their correlation to other assay endpoints

Occurrence and behavior of Dechlorane plus, Polybromodiphenyl ethers and Emerging BFRs in raptor eggs from Doñana National Park (south-western Spain)

(1,169 ± 906 ng/L) was four times higher than that in the tributary (313 ± 144 ng/L). The spatial variation of concentrations in water was associated with the emission from Dan-Shui River, the concentrations were the highest near a wastewater treatment plant (WWTP). The average concentration of BPA in the main stream of the Dan-Shui River determined to estimate the organ distribution and the bioaccumulation of these chemicals. Water, sediment and fish (Oreochromis mossambicus and Oreochromis niloticus) were collected from the Dan-Shui River. Water was pretreated with automated solid-phase extraction. Sediment and biota were extracted with matrix solid-phase dispersion. The quantification was done with ultra-high performance liquid chromatography/tandem mass spectrometry and isotope dilution techniques.

Alkylphenolic substances and BPA were detected in all of the water samples. BPA was the most abundant analyte in river water (547 ± 602 ng/L) in the tributary of the Dan-Shui River. Water was pretreated by automated solid-phase extraction. Sediment and biota were extracted with matrix solid-phase dispersion. The quantification was done with ultra-high performance liquid chromatography/tandem mass spectrometry and isotope dilution techniques.

Although BPA is easy to degrade, up to hundreds of ng/L were detected in fish. Concentrations of dechlorinating fish in organs found to be higher than that in muscle. NP was abundant in liver (3,036 ± 3,115 ng/g w.w.) and in muscle (9,597 ± 10,536 ng/g w.w.) and eggs (6,376 ± 5,142 ng/g w.w). There might be bioaccumulation of alkylphenolic substances in liver and gonad. Skewed sex ratio (femal:male = 1:7) could relate to high concentrations in the organs.

Dechloranes 602 (Dec 602), 603 (Dec 603) and 604 (Dec 604), syn- and anti-Dechlorane Plus (sDP and aDP), are halogenated flame retardants introduced as replacements for PBDEs and emerging BFRs, whereas Dechloranes were analyzed by GC-NCI-MS-MS method.

Both PBDEs and dechloranes (DP isomers, Dec 602 and Dec 603) were detected in egg samples, as well as in sediments and biota samples collected along the Doñana production facilities (China and USA), where the concentration levels of these contaminants is expected to be higher than in other places of the world. On the other hand, polybrominated diphenyl ethers (PBDEs) have been widely used as flame retardants for many years and concentration levels have been several times reported. Also, the demand for flame retardants, PBDEs are used for a wide range of consumer and industrial products in Europe. However, alternative non-BDE BSFs such as pentabromothiophenolene (PBB), hexabromobenzene (hexaBz) and decabromophenylphosphate (deBPhene) are being developed and used.

The purpose of this study was to determine the occurrence of Dechloranes, PBDEs and emerging BFRs in different raptor eggs. Eggs of white storks (Ciconia ciconia) and black kites (Milvus migrans) were collected during the breeding season of 2011. Additionally, samples of sediments, mullets (Mugil cephalus), carp (Cyprinus carpio), barbels (Loricariidae species) and red swamp crawfishs (Procambarus clarkii) were also collected for bioaccumulation and bioconcentration studies. Sample preparation methods were developed and optimized for all the flame retardants included in the study and for all the selected matrices. Instrumental determination was carried out by GC-NICI-MS for PBDEs and emerging BFRs, whereas Dechloranes were analyzed by GC-NICI-MS method.

Both PBDEs and dechloranes (DP isomers, Dec 602 and Dec 603) were detected in egg samples, as well as in sediments and biota samples collected along the Doñana National Park. The first step in the emerging contaminant levels are reported in food webs from Spain. The study of Fanti report showed a decrease in the biota samples, suggesting that syn-DP has more bioaccumulation capacity than the anti-DP.
When steroid hormones are emitted into the environment, they may have harmful effects on the reproduction system of aquatic life. Until now, research has primarily focused on human recreation, demonstrating that steroid hormones reach the aquatic environment due to insufficient removal in waste water treatment processes. However more recently, it has been revealed that agricultural practices also may add to the environmental burden of steroid hormones. So far, research Activities have mainly focused on steroid estrogens, but also androgens, progestagens and glucocorticoids, expressed in the vertebrate steroidogenesis, may occur at substantial levels in animal manure and surplus load of phosphorus handling and refined distribution of the manure nutrients to the farmlands and the possibility to reduce the environmental impact of manure nutrients, especially avoiding the surplus load of phosphorous.

In the present work we investigated the distribution of steroid hormones (pregnenolone, progesterone, dehydroepiandrosterone, androstenedione, testosterone, dihydrotestosterone, estrone, 17α-estradiol and 17β-estradiol) in raw manure and manure separates from 10 to 15 different pig farms in Denmark utilizing 4 different separation technologies. Furthermore, we investigated a possible relationship between the steroid hormone concentration and the different manure fractions and separation technologies. The steroid hormone analysis was done by inverse and integrated clean-up pressurized liquid extraction and further cleaned by a two step solid-phase extraction using adsorbers of fish, amphibians and invertebrates are also being developed in the ministry’s program. Two-tiered framework for assessing endocrine disrupting effects to organisms in the environment is being developed. This framework is designed to identify potential candidates for endocrine disruptors using available information and test results. Reliability evaluation of all data available is an important prerequisite to determine whether it might be relevant to a candidate chemicals subject to testing to assess their endocrine disrupting effects to aquatic organisms. The existing knowledge is re-evaluated to identify which in vitro assays should be conducted for prioritization to select candidate chemicals for in vivo tests. After the two batches of reliability evaluation twenty-five chemicals were identified as candidates for testing. In vitro assays were conducted for eighteen chemicals in FY 2010 and 2011 and estrogenic and anti-estrogenic activities were detected in some of them. The way of prioritized selection of chemicals subject to tier 1 in vitro testing is being discussed based on the results.

Progress and updated status of the assessment of chemicals under the EXTEND2010 will be demonstrated. In agricultural practices the animal manure can be applied to the soil as raw manure, but also as a solid or liquid manure fraction, since current livestock production facilities utilizes a developed technology which separates raw animal manure into a solid and a liquid fraction. This technology offers an improved handling and refined distribution of the manure nutrients to the farmlands and the possibility to reduce the environmental impact of manure nutrients, especially avoiding the surplus load of phosphorous.
Mo 194
Overview of available chemical analytical screening methods for identification of pollutants in European waters

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In the prevention and treatment of the disease coccidiosis, which is caused by a unicellular intestinal parasite. Coccidiosis is a major serious disease in poultry as well as in many European and intercontinental sampling and monitoring campaigns and benefit from the expertise of one of the most experienced private companies in this field. Strong networking between academia, the private sector and leading regulators in the field of river basin management and pollution management ensures the relevance of the research for practice and excellent employment opportunities for EDA-EMERGE ESRs.

Mo 195
Ionization pitfalls in nontarget screening by LC-high resolution mass spectrometry

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In nontarget screening approaches using high-resolution mass spectrometry, one important step is the determination of the molecular formula from accurate measured mass and isotope pattern. Similarly, in the suspect screening approaches the exact mass and isotope pattern of the molecular formula of the compounds of interest. In both cases the formation of protonated (positive ion mode) and deprotonated molecules (negative ion mode), is commonly anticipated when using electrospray (ESI) and atmospheric pressure chemical ionization (APCI). However, for a range of different compound classes, (de-)protonated molecules might be a minor species failing to reach selected intensity thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminants, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle.

Mo 196
RISK-IDENT: assessment of previously unknown anthropogenic trace contaminants

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For the purposes of precautionary environmental protection, the project “RISK-IDENT” develops and applies an identification system for so far unknown anthropogenic trace contaminants in the aquatic system. The development of selected trace compounds is tested in lab-scale sewage treatment plants. Column and mass spectrometry studies are used to characterise mobility. Acute and chronic effect tests will contribute to the risk assessment process. Moreover an innovative elimination method as an additional sewage treatment step based on hydroxyl radicals will be proved.

The starting point of the project is the development of a database for relevant aquatic contaminants which allows an attribution to analytical data from the analysis of real water samples. This is done by:
- Acquisition of substance data on the basis of REACH dossiers with particular reference to molecule-specific information (exact mass, log Pow, etc.) of these substances and their likely degradation products.
- Observation and application of normalised retention time factors reflecting the molecular hydrophobicity as identification criterion and allowing independent interlaboratory HPLC methods.
- Application of three different LC-MS and LC-MS/MS techniques using high-accuracy mass spectrometry for detection of contaminants via the exact mass and multiplex-reactive-monitoring (MRM) for target- and nontarget-screening strategies with low- and high-resolution tandem mass spectrometers.
- Optimisation of an procedure for identifying previously unknown trace compounds through the computer-aided comparison of analytical features with molecule-specific properties of potential water contaminants.

The poster presents the recently launched project “RISK-IDENT” and illustrates first results of the interlaboratory determination of normalised retention time factors and mass spectrometric information on the way to an independent data base applicable for all laboratories working on the water sector.

“RISK-IDENT” is supported by the German Federal Ministry of Education and Research (FKZ: 02WS1273A).

Mo 197
Detection and fate of ionophores in the environment

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Ionophores are the most heavily applied sub-group of the two sub-groups of ionophores in the environment, because they also have antibacterial properties. After the ban of antibiotic growth promoters ionophores are used extensively worldwide as prophylactic chemotherapeutics and growth promoters in livestock production. As an example, the yearly consumptions of active compounds are more than 10 tonnes in Denmark and for the Republic of Korea more than 800 tonnes. In long term, this may cause problems with resistance development in the treatment of coccidiosis. Several reports have revealed that ionophores are emerging environmental contaminants in agricultural runoff waters, surface waters, sediments, and ground waters, due to their continuously increased and constant application as feed additives in modern livestock production. Recent investigations have further reported that transformation...
products of certain veterinary drugs such as antibacterial agents (i.e. tetracyclines) possess environmental effects on the soil-bacterial community at similar level as their parent compounds. This has previously also been observed for antibacterial agents. The focus of this study is on general analytical methods for detection of ionophores and unknown transformation products in various matrices. The hyphenated method consists of an integrated clean-up with solid phase extraction followed by high-performance liquid chromatography tandem mass spectrometry (SPE-LC-MS-MS).

**References**


**MO 198**

**Prioritization of emerging pollutants on the basis of chemical structure**

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The identification of chemical compounds is a useful procedure for the identification of chemical substances and the optimization of experiments. This procedure became of particular relevance within the EU-REACH regulation, which encourages the minimization of animal testing also by the use of alternative in vitro and in silico methods. Among these methods quantitative structure-activity-relationships (QSARs) can predict missing data for the unknown activities and properties necessary to prioritize emerging contaminants. The determination of four classes of emerging pollutants (brominated flame retardants, fragrances, perfluorinated compounds and (benzo)triazoles) is one of the topics of the FP7 European project CADASTER (Case studies on the Development and Application of in-Silico Techniques for Environmental Hazard and Risk Assessment). The final goal of the project is to exemplify the integration of information, models and strategies for carrying out hazard and risk assessments for large numbers of substances, organized in the four representative chemical classes. The prioritization applied to CADASTER chemicals was crucial to focus the experimental design on critical substances on the basis of their chemical structure and potential ecotoxicological hazard. The aim of this poster is to summarize the prioritizations performed within CADASTER project, also by applying ad hoc QSAR/QSPR models developed so far (WP3) for the four classes of compounds under investigation. Different prioritization procedures were applied to over 1000 chemicals by combining, through different approaches (similarity analysis, multivariate ranking methods, factorial design), the structural information, encoded in theoretical molecular descriptors, and the data (experimental or predicted) available for different toxicological and ecotoxicological endpoints. Chemicals belonging to the ECHA pre-registration list were also studied in the prioritizations. Priority compounds were suggested for focusing the experiments executed by other CADASTER partners (WP2).

**MO 199**

**Studying nitrophenols as abiotic transformation products of phenolic microcontaminants in wastewater**

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For contaminants in wastewater, biological treatment is incomplete. Rather than removal by mineralization, Sewage Treatment Plant (STP) processes lead to the formation of transformation products through the incorporation of these compounds with the organisms in the sludge. Recent publications have classified certain transformations as “biological”, i.e. involving direct interaction with living organisms, and others as “abiotic”, implying they take place due to reactions with chemical species present in the water. A form of abiotic transformation previously observed in STPs is the nitration of phenolic contaminants, forming their corresponding nitrophenol derivatives. Nitrophenols have toxic properties. We are investigating the formation of nitrophenols further to understand both the mechanism and its occurrence in STPs. Initially, we postulate that nitration is due to the known reaction of a phenol with nitrogen dioxide (-NO2), through a radical mechanism described by Beake et al.5 The source of -NO2 is nitrite. Nitrite exists in equilibrium with its unionized form, HNO2, which decomposes slowly leading to the formation, via -NO2 of -NO.-

The nitration was first studied in batch experiments with phenol containing compounds, including morphine. The time scale of the reaction warranted the development of a fast and direct sampling and analysis method for LC/MS/MS. Although the nitration is complete within a few hours, we are able to measure its progress. The evidence suggests that it is dependent on the concentration of nitrite, the pH, and involves radical intermediates. Early experiments on morphine suggest that the formation of nitro-morphine by this reaction pathway would only occur in high-nitrite, low-pH conditions in the sludge.

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**MO 200**

**Linear solvation energy relationship models applied as classifiers in non-target analysis - a gas chromatographic approach**

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The identification of unknown substances in complex environmental mixtures plays an important role in effect-directed analysis (EDA). Our approach for the identification of unknowns is based on the generation of possible structures followed by the progressive exclusion of structures that do not match experimental chromatographic and spectral data accordingly. Linear Solvation Energy Relationships (LSERs) are applied as classifiers to predict the logarithmic retention factors log k in isocratic Gas Chromatographic (GC) measurements from the structures of candidate compounds. To demonstrate retention prediction and the application of the classifier model, twelve compounds with the molecular formula C18H17O2 were selected, while experimental log k values were compared to the predicted values and exclusion of potential candidate compounds was performed. Predicted retention factors gained from calculated structure descriptors show poor quality. Prediction was enhanced by using experimental determined descriptors, also achieved by the GC measurements.

**MO 201**

**Quantitative determination of different ether species in surface waters by Solid Phase Extraction and GC/MS**

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Numerous ether species are of growing concern to human health as well as the environment. The production and use of ethers has been rising in many industrial sectors together with the exposure of these compounds to humans. There is a common lack of available information on the use, exposure and toxicity of these compounds. In this study, a method was developed for the extraction and enrichment of six compounds from the ether family: 1,4-dioxane, monoglyme, diglyme, triglyme and tetraglyme. These compounds are of concern because they easily dissolve in water and do not partition to soils, entering ground water systems and likely contaminating public water systems. They do not break down easily and might be difficult to remove from ground water sources. Glymes are saturated polyethers which have found widespread use as enhancers of physical properties of products such as printing inks, paints, coatings and batteries. They are also commonly used as reaction solvents in the area of pharmaceuticals or specialty chemicals production. Glymes have been found to be toxic to the reproductive and/or developmental systems causing infertility and harm to the unborn child. 1,4-dioxane has been widely used as a stabilizer for chlorinated solvents. It is also utilized in products such as paint strippers, dyes and greases. Based on the available data, 1,4-dioxane is possibly carcinogenic to humans. The use of Etbe as an oxygenate gasoline additive in the production of gasoline is modest, but increasing. It has not been proven to pose any toxicity to humans.

In order to determine six ether compounds in the water samples, solid phase extraction procedure reflecting the method developed by the EPA for the determination of 1,4-dioxane in drinking water was utilized. 500 ml of a sample was passed through a charcoal containing cartridge and eluted with 50 ml of dichloromethane. All of the extracts where analyzed using a Gas Chromatography/Mass Spectrometry (GC/MS) in the selected ion monitoring (SIM) mode. To validate the method for all of the compounds a recovery study was performed, as well as a method detection limit was calculated for each ether. The same extraction procedure was used to determine the concentration of analytes in water samples in Germany. Samples from six surface water bodies (Rhein, Main, Lippe, Wesel-Datteln Canal, Schwarzbach, Auesee) in twenty four different locations were collected, extracted and analyzed.

**MO 202**

**UPLC/TOF/MS and in silico screening for transformation products of pharmaceuticals in water/sediment tests**

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Pharmaceuticals are widespread pollutants in the aquatic environment. Laboratory studies showed that the microbial community in river sediments is capable of transforming a variety of pharmaceuticals, and in some river systems this process is the dominating attenuation mechanism. In order to discriminate attenuation of pharmaceuticals along a river from dilution, suitable tools are needed. Among others, the determination of characteristic transformation products could be one such tool. The aim of this study was therefore to elucidate the transformation of several pharmaceuticals in river sediment and to evaluate this approach.

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SETAC 6th World Congress/SETAC Europe 22nd Annual Meeting