

and toxicity indicators for thousands of chemicals to be used in the USEtox model. The poster presents the methodology applied for the selection of the aquatic toxicity data available in REACH, the set of criteria used to derive various level of quality data to meet the requirement to produced Effect Factors for as many chemical as possible, and the various calculation procedure to derive final chemical effect factors. Correlation between acute and chronic toxicity for thousands of tests, for each taxonomic groups has been established, as well as the feasibility to calculate effect values based on Species sensitivity distribution. The following final calculation have been performed for thousands of chemicals: - Acute and Chronic species geometric means with standard deviation and number of individual test available per species - Arithmetic average of all the log of the species geometric mean with standard deviation and count of species as well as count of SSD group for each chemical - Lowest Acute and Chronic species geometric means with standard deviation - Comparison of the chemical toxicity based on the above calculations and chemical ranking based on GHS and CLP.

#### TU007

##### **Deriving physico-chemical input data for the USEtox model from the REACH database for thousands of chemicals using R-Studio program**

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Product Environmental Footprint (PEF) and Organisational Environmental Footprint (OEF) form a core part of the Commission Recommendation "on the use of common methods to measure and communicate the life cycle environmental performance of products and organisations" (2013/179/EU). The potential impact of chemicals emitted during the life cycle of a product is assessed *via* the USEtox multimedia fate model. This model requires for each single chemical dozens of physico-chemical parameters as well as data of ecotoxicity to freshwater aquatic life and toxicity to human for cancer and non-cancer effects. For PEF/LCA, those data are required for thousands of chemicals using the most up-to-date information. The EU commission Joint Research Centre has obtained from the chemical agency (ECHA) for more than eight thousand chemicals data regarding physico-chemical properties (166'926 test results, as of March 2017) available in the IUCLID 5.5 database. These data have been processed to automatically derive accurate values for six of the physico-chemical properties required by UseTox for fate modelling: Kow, Koc, vapour pressure, water solubility, Henry law constant and biodegradability; in addition, adsorption partition coefficient (Kd) to suspended matter, sediments and soil for inorganic compounds were determined. In order to provide high quality results, criteria were applied for selecting data on the basis of their reliability (assessed by Klimisch scores), purpose and study type. Moreover, other specific criteria were defined for each properties according to the method used, such as experimental condition (temperature and pH). Geometric mean and the coefficient of variation, for their reliability evaluation, of the consistent data selected was performed. A correlation analysis of the results with values previously included in USEtox and with values obtained with computational methods (QSAR/QSPR) was established to assess the quality of this proposed automated approach. A quality levels approach is proposed. This, paired with the abovementioned statistical index, represents a helpful support to the user for evaluating the reliability of each parameter used in the fate model. For chemicals with no available data or not satisfying the minimum quality requirements, physico-chemical properties were derived using in-silico tools (QSAR/QSPR). In particular, OECD QSAR toolbox and the EPIsuite estimation models played a fundamental role for this data gap filling purpose.

#### TU008

##### **Toward a possible Toxicity Test Battery integrated Index for Nanomaterials**

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Nanotechnology is a rapidly expanding field of research continuously producing novel materials with nanoscale properties (nanomaterials, NMs), as result, it is inevitable that NMs will enter the aquatic environment. Usually the ecotoxicological approach is generally based on a battery of bioassays with organisms belonging to different trophic levels, by choosing the appropriate endpoint for each species. While these endpoints, taken individually, can indicate the presence of a potentially deleterious effect, it is often difficult to combine these effects into an assessment of the overall status for the selected environment. Therefore is necessary to integrate all results to evaluate the risk for NMs. To synthesize the results obtained with a battery of ecotoxicological tests, different approaches were proposed. such as Toxicity test battery integrated index (TBI). This index has the advantage to put in evidence the differences between the samples. However there are still some open issues and TBI integration procedure needed to be modified according to testing sample or substance in order to represent the test sensitivity towards the matrices. In particular, when NMs are investigated also different physico-chemical behaviour and interaction with organisms should be taken into account. Therefore, the aim of this work is to study the suitability of TIB procedure for the NM to determine the needed modification for tailoring the data integration. In particular, we considered metal bearing nanoparticles (NPs) such as TiO<sub>2</sub>, SiO<sub>2</sub> and ZnO and a battery of toxicity test with organisms of different

biological complexity and representative of different trophic levels with the aim to establish a unique toxicity ranking. From the analysis of the results integration with TBI it could be highlighted that to define the hazard associated with NPs is necessary to tailor the index parameters on specific NMs physico-chemical characterization. Moreover, to make the results more reliable, together with a larger number of tests, a longer testing time for some organisms and other endpoints (genotoxic and cytotoxic parameters) should be utilized

#### TU009

##### **Historical analysis of the use of plant protection products in apple orchards (1970-2014): Combining handwritten farmers records with electronic data**

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Plant protection products (PPPs) are used to protect crops against pests and diseases and ensure yields and quality of crops. Because they are biologically active, they can cause negative side effects on the environment or humans. Data-sets on the use of PPP for specific crops over a long time would allow to get a better knowledge on the potential emissions of PPP within and beyond agro-ecosystems. However, consistent long-term datasets are mostly lacking. In addition, historic farmers' records are often only available in handwritten paper format. In Switzerland, data on PPP use in apple orchards has been voluntarily recorded by farmers since the 1950-ies, to evaluate farm economics. Up to the 1990-ies, data were only available in handwritten paper format, since 1997 they were collected electronically. In this study, we digitised the handwritten records and combined it with the electronic data. We first developed a concept, how the handwritten records can be entered into a database, which contains similar information as the electronic data. We collected data on farms (productivity), apple plantations (year of plantation, size, type, variety), and plant protection measures per plantation (product, dosage, date of application). We also developed procedures to handle missing data and to detect mistakes in the indicated dosage or field size. Finally, a dataset of spray sequences in apple orchards over the period 1970-2014 was analysed, regarding the number of treatments per PPP category (e.g. fungicides), the total amount of active ingredients applied per season and PPP category and the ranking of chemical groups per PPP category. While the average number of treatments and the average amount of active ingredients remained within a similar range, major changes were detected in the composition of applied active ingredients. For example, in the 1970-ies and 80-ies, more than 75% of all insecticide treatments were organophosphates. After 1986, organophosphates were quickly replaced by carbamates and benzoylureas, and today only contribute to about 10% of all insecticide treatments. This study illustrates, that for a historic analysis of pollutants it is sometimes unavoidable to first digitise handwritten data, because the digital revolution is a rather recent trend. This effort resulted in a unique 44 year time series of PPP use in apple orchards. In a next step, we will analyse the historic development of ecotoxicological risks of PPP usage in apple orchards.

#### TU010

##### **Using long-term datasets to assess the impacts of neonicotinoids on farmland bird populations in the UK over the last 21 years**

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Thus far the majority of research regarding neonicotinoids (NNs) has been focused on pollinator species; however, little work has been done to investigate the potential long-term impacts of these pesticides on other taxa, such as farmland birds. Birds can be directly exposed to NNs via two main exposure routes: ingestion of NN-coated grain, or seedlings germinated from coated grain. With bird abundance data, NN usage records and UK cropping data, a poisson log-linear generalised mixed model was used to investigate whether there are any impacts of NN use on farmland bird populations over a period of 21 years. Specifically, the main objectives of this study were to 1) establish whether there is a relationship between species population growth and NN usage in the UK, 2) establish whether species traits, such as body weight and home range are correlated with any effect of NNs on species population growth, and 3) to ascertain whether hypothesised exposure risk (direct) was able to explain differences between the impacts of NNs on individual species population growth. A total of 54 bird species were modelled, for which the estimated effect of NNs on population growth were highly varied. Relationships between the estimated effects and species traits, including hypothesised risk to exposure will be reported.

#### TU011

##### **Regression-based models reveal sources of pollutants in Norwegian marine sediments**

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## Research

We characterized spatial patterns of surface sediment concentrations of seven polychlorinated biphenyls (PCBs), seven polycyclic aromatic hydrocarbons (PAHs), three chlorinated pesticides and five metals in Norwegian waters and Skagerrak. In total, we analysed 5,036 concentrations of 22 chemical substances that were measured between 1986 and 2014 at 333 sampling sites by means of generalized additive models (GAMs). We found that GAMs with organic carbon content of the sediment and latitude and longitude as covariates explained ca. 75% of the variability of the contaminant sediment concentrations. For metals, a predominantly hotspot-driven spatial pattern was found, i.e. we identified historical pollution hotspots (e.g. Sjørfjord in western Norway) for mercury, zinc, cadmium and lead. Highest concentrations of PAHs and PCBs were found close to densely populated and industrialized regions, i.e. in the North Sea and in the Kattegat and Skagerrak. The spatial pattern of the PCBs suggests the secondary and diffuse atmospheric nature of their sources. Atmospheric inputs are the main sources of pollution for most organic chemicals considered, but north of the Arctic circle, we found that concentrations of PAHs increased from south to north most likely related to a combination of coal-eroding bedrock and the biological pump. The knowledge acquired in the present research is essential for developing effective remediation strategies that are consistent with international conventions on pollution control.

## TU012

### Application of a 'weight-of-evidence' model for assessing sediment quality and associated hazard with offshore gas platforms discharging produced water

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Environmental quality assessments and monitoring plans are key tools to all activities related to potential contamination of ecosystems, including marine systems. Potential effects of oil/gas production activities in Adriatic Sea (Italy) are successfully investigated since 2000 by water and sediment chemical analyses, sediment grain size analysis and bioaccumulation on native mussels. In this study, a multidisciplinary approach including chemical analyses, grain size analysis and bioassays on marine sediment, together with bioaccumulation and biomarker investigations in polychaetes exposed to sediment, is applied to assess potential impact due to offshore platforms and produced water (PFW) discharge. PFW is a complex mixture of contaminants and is the main discharge of gas/oil platforms. Marine sediment around two gas platforms (Central Adriatic region) were physico-chemically characterized by sampling of twenty-four stations at increasing distance from the platform/discharge, and in particular four stations, located at 0, 25, 50 and 100 m along the main local current, also for ecotoxicity. Different inorganic and organic contaminants were analyzed in sediment. To assess the effects of pollutants at different levels of trophic web, results of a bioassays battery composed by three different species (*Vibrio fischeri*, *Dunaliella tertiolecta*, *Tigriopus fulvus*) were considered. Moreover a battery of biomarkers at different biological levels together with bioaccumulation of some organic and inorganic contaminants were analyzed in polychaetes (*Hediste diversicolor*) exposed to sediment under laboratory conditions. A multidisciplinary weight of evidence (WOE) study was carried out, integrating different lines of evidence (LOE) as sediment chemistry, bioaccumulation, bioassays and biomarkers of four stations for each platform. These LOEs were elaborated within a quantitative WOE model which provides a synthetic hazard index for a comprehensive assessment of hazard associated to potential contaminated sediments. The WOE elaboration allowed to better summarize complex dataset of results, providing a more realistic evaluation of hazard and risk for produced water discharges.

## TU013

### Utilising biomarkers in a multispecies approach to relate organochlorine exposure and biological effects

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Due to their persistence and global distribution the use of organochlorine pesticides (OCPs) have been banned in most countries around the world. However, in a number of countries the application of DDT as malaria vector control agent is still allowed. This practice is not without controversy and reports on ecological and human health effects are increasing. The Phongolo River floodplain in north-eastern South Africa is a high risk malaria area where DDT is used as vector control agent through indoor residual spraying (IRS). This region is also regarded as a biodiversity hotspot in southern Africa and concern has been raised regarding the risk posed as a result of the long term use of DDT. Over the past seven year's studies have been undertaken to determine the degree of DDT exposure in the aquatic ecosystem through analyzing DDT and other OCP bioaccumulation in a number of different aquatic species. Concomitant biomarker analyses were

undertaken to determine the biological effect of the DDT exposure. In this poster we collated and integrated the exposure (DDT and HCH bioaccumulation) and effect (biomarker) data of the different studies to test the hypothesis that increased DDT exposure will elicit similar biological responses across species. Bioaccumulation of DDT (and its metabolites) and HCHs were measured before and after IRS application periods in two decapoda, six fish and two amphibian species. Biomarkers of exposure (cytochrome P450 and acetylcholine esterase) and effect (catalase, superoxidase dismutase, malondialdehyde, protein carbonyl, and cellular energy allocation) were analysed in the same organisms. Using principal component analysis and discriminant functional analysis the exposure and effect data were integrated to elucidate the responses of aquatic biota to OCP exposure. Although higher trophic level organisms (i.e. tigerfish - *Hydrocynus vittatus* and Müller's clawed frog - *Xenopus muelleri*) displayed the highest DDT bioaccumulation there were no distinct biomarker responses evident. When exposure data of another banned OCP,  $\gamma$ -Hexachlorocyclohexane, were included in the analysis, significant relationships with cytochrome P450 and lipid energy reserves were obtained. The result therefore indicated that biological responses were not related to DDT but rather to HCH exposure.

## Microbial community ecotoxicology in environmental risk assessment and ecosystem monitoring (P)

## TU014

### Identifying bacterial indicator taxa along an urbanization gradient in stream ecosystems

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The advent of high throughput sequencing enabled microbial eco(toxico)logists to better characterize the impact of stressors and especially pollution on microbial community structure. However, the overwhelming amount of information generated by sequencing and the high diversity of microorganisms led us to focus our analyses mainly at the community or phylum levels, ignoring all the key ecological knowledge potentially gained at the population level. In this study, we tried to move beyond beta-diversity patterns and exploit the full potential of high-throughput sequencing data by characterizing the response of individual taxa (OTUs) to a multiple stressor gradient and identifying bacterial indicator taxa. Taking inspiration from classic gradient analyses used for macro-organisms in Ecology (Threshold Indicator Taxa Analysis - TITAN, logistic and quadratic regressions), we identified bacterial taxa that presented positive, negative, neutral or subsidy-stress responses to a well characterized urbanization gradient in 41 streams in the Raleigh-Durham area (North Carolina, USA). We used a combination of environmental variables (% development, % forested, sediment Zn concentration, biotic index) that were significantly correlated to bacterial community structure to identify reliable bacterial indicator taxa along this multiple stressor gradient. Using TITAN, we identified more bacterial indicator taxa negatively impacted by urbanization than positively impacted (138 and 56 OTUs, respectively). Using quadratic regressions, we found 140 OTUs presenting a subsidy-stress response to the gradient. We observed that two bacterial families were strongly and consistently decreased by urbanization: Acidobacteriaceae (Acidobacteria) with 50% of OTUs identified as pure and reliable indicator taxa and Xanthobacteraceae (Alpha-Proteobacteria) with 39% of indicator taxa. Positive responders were distributed all over the phylogenetic tree and the family Comamonadaceae (Beta-Proteobacteria) presented the highest number of indicator taxa (14%). We calculated with TITAN that the community-level threshold, indicating the peak along the gradient where the maximum decline in all negative responders happened, was at 12.1% development. This community-level threshold occurs at very low levels of urbanization, indicating a high sensitivity of microorganisms to urbanization and the potential of bacteria to be used in bioindication or monitoring along with more traditional indexes.

## TU015

### Diuron sorption in freshwater biofilms: determination of isotherms

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In 2000, the EU Water Framework Directive (directive 2000/60/EC) was implemented with the objective of reaching the good ecological status of rivers. 45 chemicals were indexed as priority including 19 pesticides. The biofilm is at the basis of the trophic chain in aquatic environments and considered as an excellent bioindicator for water quality assessment (Edwards and Kjellerup 2013) because of its ability to integrate contamination (Vercaene-Eairmal et al. 2010). In this study, we used a photosynthesis inhibitor herbicide: diuron, one of the priority substances to the EU Water Framework Directive. Previous experiments carried out in order to characterize diuron bioaccumulation in biofilms, with two different exposure concentrations, suggest that pesticide uptake by microorganisms was not proportional to contaminant concentration in the water. For this experiment, we supposed that diuron absorption isotherms are not linear, and in order to confirm this hypothesis, bioaccumulation and toxic impact were simultaneously assessed at the equilibrium. To that aim, mature biofilm previously grown on glass slides

