Coupled modelling of plant uptake, soil water balance and soil solute transport for estimating the fate of cadmium and lead in amended agrosystems

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achieved in the area due to a shift in prescription and consumption behavior.
The effect of the scenarios is evaluated by comparison of the concentration profiles of Clarithromycin along River Main. The effect of the local technical measure at the upstream WWTP is evident from much lower simulated concentrations. The additional ozonation at another WWTP more downstream only leads to a small decrease in concentration. The regional measure proved to be much less effective in the upstream part, but results in almost the same improvement more downstream. From the simulation data at the mouth of river Main into the Rhine, it can be seen that both measures obviously removed only a small fraction of the total emission in the catchment. This is an effect of the overlying multi-point emissions from the several hundred wastewater treatment plants of which only a small number have been included in the respective measures. Concluding, the model allows for the identification of local "hot spots"and also an a priori evaluation of potential mitigation strategies. The analysis given shows that for pharmaceuticals sustainable overall reduction of surface water concentrations is hardly to be achieved by local measures, even if some of the largest WWTPs are technically refitted.

EM02B-5

Spatiotemporal exposure assessment of pesticides in flowing waters - results for predicted environmental concentrations in some brooks in Germany

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In 2011 the "Georisk"- project of the German Federal Environmental Agency was finalised. Objective of this project was to form the scientific basis for an integration of more realistic landscape based scenarios into the process of pesticide registration. Here, results of spatiotemporal simulations of PECtwa in flowing water systems are presented. The objective of the simulations was to predict initial environmental concentrations in flowing water bodies resulting from spray drift entries. Based on this the downstream development of these concentrations over space and time with regard to dispersion processes was simulated (PECtwa, Time over Threshold) including different application pattern within two days using a random generator (application time slot 2 days from 8 a.m. to 6 p.m.). We calculated 25 different application scenarios. An adequate GIS-based software-environment and a functional workflow have been developed which make use of high and medium resolution geodata (water bodies, application areas, mitigating vegetation). The observed spatial entity here is a brook in the Hallertau Region, Germany. All hydrological parameters were derived from ground truthing data. Additionally a more generalised approach using artificial scenario-based landscape definitions will also be presented.
While the risk assessment assuming lentic water bodies is based on the comparison of the PECini with the RAC, the local exposure pattern predicted by this dynamic model is summarized to the maximum TWA (i.e. 1 h, PECTWA(1h)) and the total duration when the PEC is above the RAC (ToTh). Because the local PEC is depending on the variable timing and magnitude of the pesticide entries upstream, Monte-Carlo distributions provide a set of possible exposure patterns for each segment from which different PECTWA(1h) can be extracted (e.g. minimum, maximum, median). The exposure duration (as ToTh) is based on the calculation of a RACdyn to consider that effect thresholds are higher if the exposure duration is shorter.
The results show a continuous downstream increase of ToTh and a downstream increasing TWA strongly correlated to application patterns and the hydrological parameters. The artificial scenario-based results show thresholds of hydrological parameters of the flowing water systems where the influence of the hydrological conditions are the most important influencing parameters related to the simulated PECtwa.

EM02B-6

High resolution GIS maps for predicting the POPs contamination in soil and comparison with measured data

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The assessment of POPs contamination requires reliable spatial maps for burden and flux assessment. In this work, contamination maps were developed and validated at a space resolution of 1[GREEKX]1 m with a time frame of one day, in an experimental area located in the central Alps, where direct measurements of PCB concentrations in soil and environmental parameters were available for the year 2008.
Physical algorithms calibrated on experimental data were set up for temperature and organic carbon estimation, along the soil profile and across the year, in order to deduce the horizontal, vertical and seasonal distribution of the contamination potential for PCBs in soil (Ksa maps).
The developed maps were validated with an external set of PCB contamination data, giving very good results (e.g. for CB-153, R2 = 0.80, p-value ≤ 2.2·10-06). The obtained regression coefficients were used for the mapping of the actual soil contamination (concentration maps), taking into account the temporal shifts in soil concentrations from the equilibrium (as defined by Ksa values). These maps offer the opportunity to evaluate burden and fluxes with highly resolved temporal and spatial detail, and therefore with a high degree of ecological realism (emission maps).

EM02C-1

Comparison of far field and near field exposure from consumer products for chemical exposure prioritization

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Traditionnally fate and exposure modelling for Risk Assessment and Life Cycle Assessment of products has been focusing its effort on multimedia modeling of far field exposure. However, direct exposure of consumer products via either indoor air (for e.g. indoor furniture or flooring) or via direct dermal contact (e.g. for cosmetics or toys) may represent a dominant exposure. The present project therefore aims at developing metrics and method to consistently compare near field and far field exposure to chemical in products and at testing them on a serie of case studies of three consumer products.
Direct releases from consumer products are characterized by a new metric - the Product Intake Fraction - that determines the fraction of a chemical in a product that is taken up by humans during its use and disposal phase.
Measured releases for a pacifier plasticizer used in typical average conditions leads to relatively high product intake fraction of 6·10-2 and modeled product intake fraction for different shampoo ingredients are in the range of 10-3.to 10-1 depending on the considered chemical properties. For indoor releases of the flooring material, indoor intake fraction is high in the range of 10-4.to 10-2.
Comparison between impacts of direct consumer exposure to those linked to far field life cycle emissions shows that direct impacts are of the same magnitude as or higher than indirect life cycle impacts. Similarly the impacts of indoor releases of a flooring material are of the same order of magnitude as the respiratory effects of outdoor emissions. An uncertainty analysis shows that that the extrapolation from acute to chronic toxicity was the major source of uncertainty (54.1%) and that the three main substances contributing to the impacts also dominated the uncertainty with 84.0% of the total uncertainty.

EM02C-2

Assessment of local impacts of municipal solid waste management using life cycle assessment (LCA)

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This research takes part in a PhD work whose aim is to develop a methodology to assess locally environmental impacts of municipal waste management (MSW) in order to provide environmental elements to local decision makers and stakeholders.
MSW is a local issue managed under the responsibility of local authorities. To integrate environmental considerations, decision-makers often use Life Cycle Assessment (LCA). However, the LCA methodology does not take into account the characteristics of the territory involved and consequently not allow local assessment. Nevertheless, such a consideration appears necessary for local issues such as toxicity and odours. To solve the problem of assessing local impacts, the SETAC (Society of Environmental Toxicology and Chemistry) recommends the use of the Site dependent approach. This approach allows considering, in the characterization step, some spatial and temporal conditions of releases and some characteristics of the potentially affected environment in order to realize fate, exposure and effect analysis.
Our methodological research focuses on fate analysis step and its integration in the classification step. The novelty of our approach is the consideration of local environmental characteristics, through the USEtox model in a modified version, to locally assess toxicity and odours impacts. USEtox is a multimedia model which describes the fate, the exposition and the effect of substances released in the environment through three boxes (global, continental and urban). For spatial assessment of substances fate, we propose to change in the dimensions of the environmental boxes, compartments and in local relevant parameters which are determined by default in USEtox and not suitable for local assessment.
This work leads to the construction of a new set of spatial elements for classification and characterization steps for toxicity and odours impacts. The new classification step will be based on USEtox results from the new version and the consideration of spatiotemporal conditions of emission. The characterization step will be limited to the consideration of health effect and olfactory thresholds. The final objective is to compare classical LCA results (without taking into account spatial and temporal parameters) with located toxicity and odour LCA results. The spatial assessment of local impacts should allow policy makers and stakeholders to get "personalized"answers to debate within the decision-making.

EM02C-3

Coupled modelling of plant uptake, soil water balance and soil solute transport for estimating the fate of cadmium and lead in amended agrosystems

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Soil water balance, solute transport, leaching to groundwater and plant uptake of solute and water are coupled processes. Recently, a coupled plant and groundwater transport model for NaCl could simulate the transpiration-induced changes in groundwater salinity. However, for metals, no models that simultaneously predict plant uptake as well as leaching to groundwater were found. In this study, the water budget of soil, the uptake into plants and the leaching to groundwater of cadmium (Cd) and lead (Pb) were simulated simultaneously using a physiological plant uptake model and a tipping buckets water and solute transport model for soil.
Factors affecting uptake of trace metals into vegetation are type of metal, plant species and cultivar, plant-related parameters such as transpiration and growth, and soil parameters like pH, organic matter, soil texture and redox status. Robust tools for predicting the transfers of metals from soil and air to plants are scarce and often incorrect due to the large variability of metal uptake in plants.
The objective of this work is to present and test a model framework for the simulation of the coupled transport of water and dissolved trace metals, the uptake of both into crops, and leaching of solute and water to groundwater. The model is parameterized with data derived from a ten-year field study where four organic amendments were applied every two years.
Simulation results were tested on measured concentrations of lead (Pb) and cadmium (Cd) in soil and plants from the ten-year field study. Predicted concentrations slightly decreased with time in control soils, but increased in amended soils by about 10% (Cd) and 6% to 18% (Pb). Estimated plant uptake was lower in amended plots, due to an increase of Kd. Predicted concentrations in plants were close to measured levels in plant residues (straw), but higher than measured concentrations in grains. Initially, according to the model, lead was mainly deposited from air into plants (82% in 1998); later uptake from soil was dominating (30% from air in 2006), because of decreasing levels in air. For cadmium, uptake from air into plants was negligible (1-5%).

EM02C-4
Ranking of emissions of plant protection products from protected crops to environmental receptors
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A number of EU Member States requested EFSA to develop guidance on how to carry out environmental risk assessment of Plant Protection Products (PPPs) emitting from covered crops. In response, EFSA established a working group and commissioned supporting research to establish an inventory of protected crop systems and to determine the importance of emissions from these systems to relevant environmental compartments. The working group developed a classification system, consisting of 13 categories ranging from mulching and direct cover to high-tech greenhouses and closed buildings, in order to categorise the enormous variability in covered crop systems. The work on emissions performed so far revealed that emissions from covered crops may be substantial and might have been underestimated in the past. For the small and more open systems, it is expected that emissions do not substantially differ in comparison to open field systems. Comparison of emissions from selected closed walk-in structures with emissions from open field identified greenhouses and walk in tunnels having priority for scenario development for risk assessment. For these covered crop systems, the Panel on Plant Protection products and their Residues (PPR Panel) recommends the development of tiered risk assessment procedures. Further investigation is necessary to find out whether risk assessment for open field may be used as the first tier in these procedures. Furthermore, elements were identified that should be considered in deriving the risk assessment scenarios, for both soil-bound and soil-less cultivations.

EM02C-5
EU scenarios for exposure of soil organisms resulting from spray applications of pesticides to annual crops
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Based on a Member State consultation EFSA initiated a revision of the guidance for the soil exposure assessment including development of EU scenarios for numerical models. The aim of the exposure assessment was to obtain a 90th percentile of the PEC in space and time considering all fields in the regulatory zones North, Centre and South grown with the target crop where this active substance is applied. The types of ecotoxicologically relevant concentrations considered were both the concentration in total soil and the concentration in pore water averaged over the top 1, 2.5, 5 or 20 cm of soil (both peak and TWA concentrations for time windows up to 56 d). The scenario selection was based on a simple analytical model that calculates the concentration in soil assuming that degradation (first-order kinetics at a constant rate) is the only loss process from the 20-cm plough layer. The concentration in the pore water was calculated assuming a linear sorption isotherm assuming that sorption is proportional to organic matter. Concentration maps were calculated at a resolution of 1x1 km2 for the whole area of annual crops in each of the regulatory zones North, Centre and South. Simulations including uncertainty in the dry bulk density and in substance properties such as the Kom and the DegT50 showed that a spatial 95th percentile has to be selected for obtaining an overall 90th percentile when median or geomean values of these substance properties are used as input for the scenario calculations in the regulatory process. So the target was to select a spatial 95th percentile. Scenario were selected based on maps of the peak concentrations in total soil and in pore water that were generated for 19 substances and averaging depths of 1 and 20 cm. The selected scenarios for concentration in total soil have all relatively high organic matter contents and low temperatures. However, the selected scenarios for the pore water concentration have all relatively low organic matter contents because the pore water concentration is almost directly proportional to the inverse of the organic matter content for substances that show significant sorption. Calculations with the simple analytical model for a number of example substances showed that the concentration in total soil increased in the order South-Centre-North and that the concentration in the pore water increased in the order North-Centre-South (so opposite orders for these two types of concentration).

EM02C-6
Mechanisms behind conservatism in tiered soil risk assessment
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In recent EFSA opinions on assessment of exposure of organisms to substances in soil a rigorous scientific concept was presented to describe the spatio-temporal distribution of chemical substances in soil. Further ecologically relevant soil layers were derived. These layers represent the habitat of specific soil organisms used for risk assessment. For example the soil layer 0 1 cm is proposed for epigeic and anecic earthworms. The mean concentration for this layer (**E**cologically **R**elevant **C**oncentration) can be identified from the predicted concentration depth distribution. It is finally used for lower tier risk assessment (RA) in combination with an effect endpoint, e.g. a NOEC.
Though this approach appears straightforward it produces a surprising result. Compared to current soil RA it leads to dramatically increased ERC for a number of test organisms. On the other hand there are several publications comparing the current lower tier soil RA to higher tier (field) studies serving as reference tier. These came to the conclusion that the current soil RA is appropriate, i.e. it discriminates between critical and uncritical substances in sufficiently conservative way.
Why does the soil RA proposed by EFSA become so conservative and is this justified? A concept is proposed which analyses the whole process (design of lower tier effect study, derivation of endpoint, link to the exposure situation under real-world conditions) in order to provide answers to the above question.
The RA for earthworms is used as example because of the large number of studies available. Several factors may be considered to attribute to the different occurrence of effects in lower (lab) and reference tier (field) studies.
- Time to effect. Duration of study at reference tier typically 1 year, usually 56 days at lower tier (earthworm reproduction).
- Likeliness of proposed ecologically relevant soil layer, e.g. 0-1 cm. This habitat is very narrow. Extremes of soil moisture and temperature may render it temporarily to a hostile environment
- Impact of initial concentration. NOEC values usually in terms of initial concentration. Often experimental period at reference tier is long compared to DT50 of compound. Thus mean concentration is likely to be much lower than initial one.
These factors are investigated employing detailed analysis of the spatio-temporal concentration distribution in soil. Based on this information local effects can be estimated and aggregated on population level.

EM02D-1
Variability and estimation of pesticide half-lives in vegetation
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