chemicals, pesticides, and pharmaceuticals. The effects of these compounds on gene and protein expression in multiple cell lines are evaluated via 700 bioassays. The unprecedented collection of toxicological data is ideal for *in silico* elucidation of toxicity mechanisms and AOPs. We identified all ToxCast assays pertaining to the Nrf2 OS-response pathway and evaluated the relationships between electrochemical parameters and Nrf2 response pathway, as evaluated by ToxCast . Several bZip transcription factors exhibit patterns of expression similar to Nrfw. Furthermore, the activity of chemicals activating multiple bZip factors tends to lie outside the region of general cytotoxicity and burst effects. The patterns of pathway-specific gene expressions observed in ToxCast and the relationship with reactivity and shaper parameters will help unravel the diverse network. The Molecular Design Research Network (MODRN) aims to use the property-effect relationships and advanced modeling and machine learning techniques to create design guidelines for minimizing oxidative stress effects generate by commercial chemicals.

WE320

Comparison of Ready Biodegradation Estimation Methods for Fragrance Materials and Application to Musks

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Biodegradability is fundamental to the assessment of environmental exposure and risk from organic chemicals. Predictive models can be used to pursue chemical design (green chemistry) objectives, which are most effectively met when models are easy to use and available free of charge. The objective of this work was to evaluate no-cost estimation programs with respect to prediction of ready biodegradability. Fragrance materials, which are structurally diverse and have significant exposure potential, were used for this purpose. Using a database of 222 fragrance compounds with measured ready biodegradability, 10 models were compared on the basis of overall accuracy, sensitivity, specificity, and Matthews correlation coefficient (MCC). The 10 models were VEGA© Non-Interactive Client, START (Toxtree©), Biowin©1–6, and two models based on inductive machine learning. Applicability domain (AD) was also considered. Overall accuracy was ca. 70% and varied little over all models, but sensitivity, specificity and MCC, showed wider variation. Based on MCC, the best models for fragrance compounds were Biowin6, VEGA and Biowin3. VEGA performance was slightly better for the compounds it identified as having “high reliability” predictions (AD index >0.8). However, removing compounds with one and only one quaternary carbon yielded a similar improvement in predictivity for VEGA and Biowin3/6, but with a smaller penalty in reduced coverage. Results from the models were then used to compare musks across the various structural classes and make inferences about their environmental attributes.

WE321

Substitution of long chain fluorinated copolymers for durable water repellent (DWR) textile modification

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Fabric`s repellency against polar and non-polar liquids while maintaining breathability is a key functionality in modern textiles. Durable water repellent (DWR) polymers can provide these properties and are therefore produced in high tonnages. Despite differences in polymer architecture that mainly depend on end-uses in textiles, all state of the art DWR polymers have hydrophobic side chains linked to a polymer backbone. These non-polar side chains are based on hydrocarbons, silicones or perfluorinated (PF) moieties and need to be closely packed and orientated towards the fiber surface to achieve an “umbrella-like” repellent effect. Textiles treated with these polymers however might be a source of leaching chemicals caused by degradation of the polymeric (non-fluorinated) backbone or the release of impurities (from production) during the life cycle of textiles. Considering worst case scenarios, degradation can result in persistent contaminants which have been found in textiles already. The phase-out of persistent, bioaccumulative and toxic long chain PF raw materials that were used for very effective DWRs in the past resulted in the development of alternatives based on short chain fluorocarbons (C6 and C4). Although these side chain fluorinated polymers can be considered less toxic and less bioaccumulative, their potential to form mobile and persistent contaminants is not fully understood. Other “ecofriendly” DWR technologies based on silicones or novel star-shaped hydrocarbons (dendrimers) have unclear degradation pathways as well. This lack of reliable data makes a corresponding risk assessment impossible. The aim of the interdisciplinary collaboration SUPFES (http://www.supfes.eu/) is to help industry in finding alternatives that can replace long-chain fluorocarbons in textiles with environmentally more benign alternatives. Within the project a unique consortium of scientific and industrial partners collaborate to make sure that functionality and environmental impact can be balanced in the design of future DWR products.

WE322

Aquatic toxicity of biofuels - Using ecotoxicological methods for sustainable biofuel development

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The increasing global demand for energy, e.g., for the fossil fuel-dominated transport sector requires the development of alternative energy sources. Due to declining production capacities and environmental concerns of fossil fuels, such as emissions of greenhouse gases, governmental support for the development of renewable energy sources, such as biomass-derived fuels, increased considerably. A rise in biofuel production and consumption increases the risk of a release into the environment. The lack of ecotoxicological data on biofuels impedes a sufficient assessment of their environmental hazard potentials. Ecotoxicological biotests can be applied in a prospective assessment of the hazard potential for aquatic ecosystems and allow an identification of the most environmentally friendly biofuel even at a very early stage of the development. This study focused on the investigation of one potential biomass-derived fuel candidate, 2-methyltetrahydrofuran (2-MTHF). The ecotoxicological investigation was conducted by means of acute and chronic *Daphnia magna* biotests according to OECD 202 und OECD 211 adapted to the testing of biofuels, as well as a *Daphnia magna* population assay. We used a toxicokinetic-toxicodynamic (TKTD) model to describe the process leading to a toxic effect and subsequently integrated this model into an individual-based population model. This allows for the extrapolation of population level effects from individual-toxicity testing. The TKTD model is deemed suitable to describe effects resulting from time-variable exposure of the volatile substance. Results from ecotoxicological biotests were used to inform the process-based effect model. Modell predictions at the population level were tested along independent population data. This evaluation reveals that the methods applied can be used in a sustainable biofuel development to assess the effects on a population level. However, testing of further potential biofuels has to be conducted.
Acknowledgement: This work was performed as part of the Research Cluster "Tailor-made fuels from biomass", which is funded by the Excellence Initiative by the German federal and state governments to promote science and research at German universities.

Challenges of regional and global modelling nitrogen and phosphorus in agriculture supply chains (P)

WE323

Macroalgae production and biorefining in Denmark - a life cycle assessment

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Macroalgae is a key biomass for the future development of a biobased society. A model of the brown algae *Saccharina latissima* is here utilized as feedstock for a biorefinery system which produces bioethanol, proteins and fertilizers. A Life Cycle Assessment was conducted from cradle to grave; i.e. from cultivation and harvest of *Saccharina latissima* in Limfjorden in the North of Jutland in Denmark, to the use and disposal of the products. The system boundary includes transport and stepwise bioconversion into the above mentioned bioproducts, using system expansion to take into account ecosystem services delivered by the system. The analysis shows that the productivity of the macroalgae dramatically affects the environmental sustainability of the biorefinery system quantified by the impact categories: Climate Change, Marine Eutrophication and Marine Ecotoxicity. Results of the study reveal the use of macroalgae as instrument for reduction of marine eutrophication by P and N fixation when nutrients are then applied in agricultural soil. Carbon and nitrogen flow within the system boundary are quantified and described showing an increase in the soil carbon stock corresponding to a net reduction of CO_2 in the atmosphere.

WE324

Modelling the nitrogen balance of tropical perennial crops: state of the art and challenges for oil palm plantations

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While a number of models exist to estimate nitrogen (N) losses from agricultural fields, they mostly pertain to temperate climate conditions and annual crops. Few models are available for tropical crops [1], [2], and even fewer for perennial crops [3], [4]. The lack of robust N-flux inventories is particularly critical for LCA of perennial and tropical crops. Oil palm is the most rapidly expanding tropical perennial crop, which raises environmental concerns. Beside land-use change and peatland, oil palm agricultural production impacts the environment mainly through the use of synthetic fertilisers, notably nitrogen [5], [6]. The latter is associated with pollution risks of ground and surface water, and emissions of greenhouse gases. Accurate estimation of N losses is critical to assess the environmental impacts of palm plantations. In this study, we reviewed currently-available models for oil palm cultivation, and appraised their capacity to assess the N balances of oil palm agro-ecosystems. We identified various operational and process-based models that could be applied to oil palm, although most of them were not specifically adapted for tropical perennial crops. To our knowledge, APSIM is the only available process-based model of oil palm cultivation that includes N losses [7], but the accuracy of its N loss estimates was untested. Other means of assessment were based on statistical models [8]–[10] or other approaches [11]–[13]. Nitrogen balance assessments have shown important uncertainties (Figure). Estimates of N_20 and NO_3^- rely on very uncertain and sensitive parameters, such as the clay content for instance with the SQCB-NO3 model [13]. These uncertainties are due to a lack of understanding of processes. In particular, it is difficult to study and understand N dynamics over the whole lifespan of oil palm crops (20-25 years) and to account for varying agricultural practices. Adequate data to characterise various cropping systems is often lacking. Further research is required to develop a procedure that provides a robust assessment of the environmental impact of N management in oil palm cultivation. Particularly, this procedure should have the capacity to account for a range of soils, climates, and management practices over the whole cycle. One track to be pursued is the development of an agro-ecological indicator based on Indigo concept [14], [15]. Such an indicator could help to reduce uncertainties in LCA of tropical perennial crops.

WE325

Quantifying within-farm nitrogen and phosphorus efficiency in grazing-based dairy production systems

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The ongoing trend for increased intensification is occurring in grazing-based, as well as confinement-based dairy farms, worldwide. Grazing-based dairy farms are increasingly reliant on imported feed and fertiliser, with consequent greater nitrogen (N) and phosphorus (P) flows, transformations and losses, and a decreasing dependence on N inputs from N_2 fixation by pasture legumes. While it is important to understand how much N and P is imported and subsequently removed in product on dairy farms, the ability to quantify within-farm flows and transformations, as well as the spatial and temporal distribution of N and P, is essential to identify opportunities for improved management. The purpose of this paper is to outline key components of N and P flows and transformations within grazing-based dairy operations, and propose simple metrics which can be used to quantify N and P use efficiencies and manure management practices, using readily collected information from dairy farms. The linking of farm-gate balances with internal N and P cycling processes provides opportunities for targeted improvements in N and P capture and recycling by farmers, and reducing losses of N and P from grazed dairy systems. In particular, this should include: (i) quantifying key nutrient inputs, outputs and stores (i.e. feed, manure) and nutrient balances and efficiencies at a simple (farm-gate) level, (ii) quantifying grazing animal N and P intakes and feed N and P use efficiencies, at least within each season, (iii) quantifying N and P distribution and loading rates at a paddock management scale, including inputs and outputs such as fertiliser applications, forage removal, and importantly grazing animal excreted N and P, and (iv) quantifying the amount and proportion of excreta N and P deposited in unproductive areas which go uncollected, as well as the amount and proportion of excreta N and P collected and redistributed. Such information from suitably comparable farms, can be used to benchmark farms across a range of indices and target farm management improvements. These data targeting within farm spatial and temporal variability need to be factored into LCA studies conducted on grazing based dairy farm systems to more effectively describe the effectiveness of N and P recycling and loss.

Prospective Life Cycle Thinking approaches for the definition and implementation of sustainability strategies in industry and policy making (P)

WE326

Prospective LCA for the implementation of an innovating technology recovering nutrients from urine

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The risk of phosphorous depletion and of ore quality decrease in the coming future and the increased energy requirements for nitrogen production make urine, where these compounds are highly concentrated, an interesting resource and call for efficient nutrients recovery process. The ValuefromUrine project (FP7 funding) aims at developing a new urine treatment technology based on an energy-efficient bio-electrochemical system. Life Cycle Assessment (LCA) is used to evaluate the overall environmental impacts and benefits of the technology, including its infrastructures and operation, the sewer network where treated urine is mixed with wastewater from other sources and the effects on wastewater treatment plants. The performance of the technology is expected to evolve during the project duration, from the lab tests to a prototype demonstrating its functioning. This emerging technology could be even implemented at larger scale in the market. As a result, life cycle inventory data can be largely affected by these scale changes, both at the foreground and background levels, and by technology evolution in the supply chain. The intended approach to tackle this issue is the definition of prospective scenarios based on Formative Scenario Analysis (FSA). First, the system is modelled to calculate the inventory data based on parameters, which can be either fixed (e.g. chemical properties) or variable (e.g. urine flow); and related to design choices (e.g. size of the cell components) or uncontrolled by the operator (urine composition). They constitute the technological impact variables (system element influencing the system behaviour), which are then completed by socio-economic impact variables for the FSA. The relations and effects between impact variables are assessed in an impact matrix to identify the key variables. The future state of each key variable is estimated (including uncertainty distributions whenever possible) according to three scenarios: low, medium and large deployment of the technology (e.g. the more the technology is deployed, the larger is the scale, the more efficient it should be). Inventory data can finally be modelled for the different scenarios, allowing the calculation of the life cycle environmental impacts. The latter are represented through uncertainty distributions for the different deployment scenarios and are compared to the scenario without the technology (urine is directly sent to sewer network without pre-treatment).

WE327

Energy Recovery from wastewater Treatment Plants in Scotland: A Life cycle Analysis Approach

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Waste streams with calorific or resource value exist across all sectors of industry. Currently, many of these streams go to sewer or landfill. There is a vast potential to use such waste streams for renewable energy generation, especially within the water industry. The entire UK Water Industry uses a total of 7,703 GWh/year in electricity whilst Scottish Water currently consumes around 450 GWh/year of electricity. Energy used on clean water production is predicted to decrease in response to leakage and demand reduction, whilst wastewater treatment is likely to show a significant increase due to water quality drivers. Energy recovery strategies could help offset the electricity consumption of the wastewater sector and represent possible areas for sustainable energy policy implementation. In Scotland, many diverse strategies are in place to improve the quality of wastewater treatment, but unfortunately the more advanced the treatment, usually the more energy is required in order to produce better effluent quality. This necessitates a robust energy reduction strategy for the sector, but attaining the required level of water quality and energy savings can be associated with other environmental costs such as emissions from energy production and increase in runoff from sludge application to land. The goal of this study is to investigate both upstream and downstream opportunities for reducing or offsetting energy demand and report on potential energy savings and recovery from wastewater treatment plants in Scotland with its associated costs. Preliminary investigations suggest that the application of sludge to derelict lands for dedicated energy crops production, which as biogas can generate electricity and heat is a potential route for energy recovery. The project uses data from surveys of treatment plants, from site visits to selected facilities, from equipment suppliers, and from published technical literature to analyse the potential for energy recovery. Life Cycle Assessment (LCA) has been the analytical tool used to evaluate environmental loadings. Initial results from the analysis of the selected systems will be presented and analytic issues will be discussed, including an approach to derive budgets of water and energy inputs for water and waste processing, P stocks and flows. The project will be extended to evaluate implications of projections of population, energy and water demand for future energy costs associated with water supply and treatment.

WE328

From waste to product: a paradigm shift in Life Cycle Assessment applied to wastewater sewage sludge

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Since the last 20 years, wastewater treatment plants are become more effective in releasing a good quality water in the ecosystem due to stringent European directives aiming at maintaining and improving the aquatic environment (Directive 91/271/EEC, Directive 2000/60/EC). As a consequence, huge amount of wastewater sewage sludge are produced each year. This sludge is currently considered as a waste but new industrial practices and european regulation (End-of-Waste directive) are ongoing to consider sludge as a valuable product. In Life Cycle Assessment (LCA), boundarie are well drawn up between LCA of products and LCA of waste management. Indeed, LCA of products takes into consideration the whole product life cycle from the raw material extraction up to the product end of life with a functionnal unit defined in terms of system's output (i.e. the product). LCA of waste management considers one or several wastes entering the system from the moment it becomes a waste by loosing value up to the moment it regains value or leave the waste management system as an emission. Specificities of this type of LCA are twofold (1) a functionnal unit defined as a system's input (the waste to be treated) and (2) the assumption that the waste is free of any environmental load when entering the system, assumption often known as the "zero burden approach". So there is an important gap between the two types of LCA. If