A Quantitative Property-Property Relationship for the Internal Diffusion Coefficients of Organic Compounds in Solid Materials

Indoor releases of organic chemicals encapsulated in solid materials are major contributors to human exposures and are directly related to the internal diffusion coefficient in solid materials. Existing correlations to estimate the diffusion coefficient are only valid for a limited number of chemical-material combinations. This paper develops and evaluates a quantitative property-property relationship (QPPR) to predict diffusion coefficients for a wide range of organic chemicals and materials. We first compiled a training dataset of 1103 measured diffusion coefficients for 158 chemicals in 32 consolidated material types. Following a detailed analysis of the temperature influence, we developed a multiple linear regression model to predict diffusion coefficients as a function of chemical molecular weight (MW), temperature, and material type (adjusted R2 of 0.93). The internal validations showed the model to be robust, stable and not a result of chance correlation. The external validation against two separate prediction datasets demonstrated the model has good predicting ability within its applicability domain (R2ext > 0.8), namely MW between 30 and 1178 g/mol and temperature between 4 and 180 °C. By covering a much wider range of organic chemicals and materials, this QPPR facilitates high-throughput estimates of human exposures for chemicals encapsulated in solid materials.
Sensitivity-based research prioritization through stochastic characterization modeling

Product developers using life cycle toxicity characterization models to understand the potential impacts of chemical emissions face serious challenges related to large data demands and high input data uncertainty. This motivates greater focus on model sensitivity toward input parameter variability to guide research efforts in data refinement and design of experiments for existing and emerging chemicals alike. This study presents a sensitivity-based approach for estimating toxicity characterization factors given high input data uncertainty and using the results to prioritize data collection according to parameter influence on characterization factors (CFs). Proof of concept is illustrated with the UNEP-SETAC scientific consensus model USEtox.

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A review of models for near-field exposure pathways of chemicals in consumer products

Exposure to chemicals in consumer products has been gaining increasing attention, with multiple studies showing that near-field exposures from products is high compared to far-field exposures. Regarding the numerous chemical-product combinations, there is a need for an overarching review of models able to quantify the multiple transfers of chemicals from products used near-field to humans. The present review therefore aims at an in-depth overview of modeling approaches for near-field chemical release and human exposure pathways associated with consumer products. It focuses on lower-tier, mechanistic models suitable for life cycle assessments (LCA), chemical alternative assessment (CAA) and high-throughput screening risk assessment (HTS). Chemicals in a product enter the near-field via a defined "compartment of entry", are transformed or transferred to adjacent compartments, and eventually end in a "human receptor compartment". We first focus on models of physical mass transfers from the product to 'near-field' compartments. For transfers of chemicals from article interior, adequate modeling of in-article diffusion and of partitioning between article surface and air/skin/food is key. Modeling volatilization and subsequent transfer to the outdoor is crucial for transfers of chemicals used in the inner space of appliances, on object surfaces or directly emitted to indoor air. For transfers from skin surface, models need to reflect the competition between dermal permeation, volatilization and fraction washed-off. We then focus on transfers from the 'near-field' to 'human' compartments, defined as respiratory tract, gastrointestinal tract and epidermis, for which good estimates of air concentrations, non-dietary ingestion parameters and skin permeation are essential, respectively. We critically characterize for each exposure pathway the ability of models to estimate near-field transfers and to best inform LCA, CAA and HTS, summarizing the main characteristics of the potentially best-suited models. This review identifies large knowledge gaps for several near-field pathways and suggests research needs and future directions.

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan, National Risk Management Research Laboratory
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Ecological and human health risks associated with abandoned gold mine tailings contaminated soil

Gold mining is a major source of metal and metalloid emissions into the environment. Studies were carried out in Krugersdorp, South Africa, to evaluate the ecological and human health risks associated with exposure to metals and metalloids in mine tailings contaminated soils. Concentrations of arsenic (As), cadmium (Cd), chromium (Cr), cobalt (Co), copper (Cu), lead (Pb), manganese (Mn), nickel (Ni), and zinc (Zn) in soil samples from the area varied with the highest contamination factors (expressed as ratio of metal or metalloid concentration in the tailings contaminated soil to that of the control site) observed for As (3.5x10²), Co (2.8x10²) and Ni (1.1x10²). Potential ecological risk index values for metals and metalloids determined from soil metal and metalloid concentrations and their respective risk factors were correspondingly highest for As (3.5x10³) and Co (1.4x10³), whereas Mn (0.6) presented the lowest ecological risk. Human health risk was assessed using Hazard Quotient (HQ), Chronic Hazard Index (CHI) and carcinogenic risk levels, where values of HQ > 1, CHI > 1 and carcinogenic risk values > 1×10⁻⁴ represent elevated risks. Values for HQ indicated high exposure-related risk for As (53.7), Cr (14.8), Ni (2.2), Zn (2.64) and Mn (1.67). Children were more at risk from heavy metal and metalloid exposure than adults. Cancer-related risks associated with metal and metalloid exposure among children were also higher than in adults with cancer risk values of 3×10⁻² and 4×10⁻² for As and Ni respectively among children, and 5×10⁻³ and 4×10⁻³ for As and Ni respectively among adults. There is significant potential ecological and human health risk associated with metal and metalloid exposure from contaminated soils around gold mine tailings dumps. This could be a potential contributing factor to a setback in the health of residents in informal settlements dominating this mining area as the immune systems of some of these residents are already compromised by high HIV prevalence.

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Exploring REACH as a potential data source for characterizing ecotoxicity in life cycle assessment

Toxicity models in life cycle impact assessment (LCIA) currently only characterize a small fraction of marketed substances, mostly because of limitations in the underlying ecotoxicity data. One approach to improve the current data situation in LCIA is to identify new data sources, such as the European Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH) database. The present study explored REACH as a potential data source for LCIA based on matching reported ecotoxicity data for substances that are currently also included in the United Nations Environment Programme/Society for Environmental Toxicology and Chemistry (UNEP/SETAC) scientific consensus model USEtox for characterizing toxicity impacts. Data are evaluated with respect to number of data points, reported reliability, and test duration, and are compared with data listed in USEtox at the level of hazardous concentration for 50% of the covered species per substance. The results emphasize differences between data available via REACH and in USEtox. The comparison of ecotoxicity data from REACH and USEtox shows potential for using REACH ecotoxicity data in LCIA toxicity characterization, but also highlights issues related to compliance of submitted data with REACH requirements as well as different assumptions underlying regulatory risk assessment under REACH versus data needed for LCIA. Thus, further research is required to address data quality, pre-processing, and applicability, before considering data submitted under REACH as a data source for use in LCIA, and also to explore additionally available data sources, published studies, and reports.

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IMPROVING SUBSTANCE INFORMATION IN USETOX®, PART 1: DISCUSSION ON DATA AND APPROACHES FOR ESTIMATING FRESHWATER ECOTOXICITY EFFECT FACTORS: Effect factor in USETOX

The scientific consensus model USEtox® is recommended by the European Commission as the reference model to characterize life cycle chemical emissions in terms of their potential human toxicity and freshwater aquatic ecotoxicity impacts in the context of the International Reference Life Cycle Data System (ILCD) Handbook and the Environmental Footprint pilot phase looking at products (PEF) and organisations (OEF). Consequently, this model has been systematically used within the PEF/OEF pilot phase by 25 EU industry sectors, which manufacture a wide variety of consumer products. This testing phase has raised some questions regarding the derivation of and the data used for the chemical-specific freshwater ecotoxicity effect factor in USEtox®. For calculating the potential freshwater aquatic ecotoxicity impacts, USEtox® bases the effect factor on the chronic hazard concentration (HC50) value for a chemical calculated as the arithmetic mean of all logarithmized geometric means of species-specific chronic lethal (or effect)
concentrations (L(E)C50). We investigated the dependency of the USEtox® effect factor on the selection of ecotoxicological data source and toxicological endpoints, and we found that both influence the ecotoxicity ranking of chemicals and may hence influence the conclusions of a PEF/OEF study. We furthermore compared the average measure (HC50) to other types of ecotoxicity effect indicators like the lowest species EC50 or NOEC, frequently used in regulatory risk assessment, and demonstrated how they may also influence the ecotoxicity ranking of chemicals. We acknowledge that these indicators represent different aspects of a chemical's ecotoxicity potential and discuss their pros and cons for a comparative chemical assessment as performed in LCA and in particular within the PEF/OEF context. This article is protected by copyright. All rights reserved.

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Stochastic modeling of near-field exposure to parabens in personal care products

Exposure assessment is a key step in determining risks to chemicals in consumer goods, including personal care products (PCPs). Exposure models can be used to estimate exposures to chemicals in the absence of biomonitoring data and as tools in chemical risk prioritization and screening. We apply a PCP exposure model based on the product intake fraction (PiF), which is defined as the fraction of chemical in a product that is taken in by the exposed population, to estimate chemical intake based on physicochemical properties and PCP usage characteristics. The PiF can be used to estimate route and pathway-specific exposures during both the use and disposal stages of a product. As a case study, we stochastically quantified population level exposures to parabens in PCPs, and compared estimates with biomarker values.

We estimated exposure based on the usage of PCPs in the female US population, taking into account population variability, product usage characteristics, paraben occurrence in PCPs and the PiF. Intakes were converted to urine levels and compared with National Health and Nutrition Examination Survey (NHANES) biomonitoring data. Results suggest that for parabens, chemical exposure during product use is substantially larger than environmentally mediated exposure after product disposal. Modeled urine concentrations reflect well the NHANES variation of three orders of magnitude across parabens for the 50th, 75th, 90th, and 95th percentiles and were generally in good agreement with measurements, when taking uncertainty into account. This study presents an approach to estimate multi-pathway exposure to chemicals in PCPs and can be used as a tool within exposure-based screening of chemicals as well in higher tier exposure estimates.

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Towards harmonizing natural resources as an area of protection in life cycle impact assessment

In this paper, we summarize the discussion and present the findings of an expert group effort under the umbrella of the United Nations Environment Programme (UNEP)/Society of Environmental Toxicology and Chemistry (SETAC) Life Cycle Initiative proposing natural resources as an Area of Protection (AoP) in Life Cycle Impact Assessment (LCIA).

As a first step, natural resources have been defined for the LCA context with reference to the overall UNEP/SETAC Life Cycle Impact Assessment (LCIA) framework. Second, existing LCIA methods have been reviewed and discussed. The reviewed methods have been evaluated according to the considered type of natural resources and their underlying principles followed (use-to-availability ratios, backup technology approaches, or thermodynamic accounting methods).

There is currently no single LCIA method available that addresses impacts for all natural resource categories, nor do existing methods and models addressing different natural resource categories do so in a consistent way across categories. Exceptions are exergy and solar energy-related methods, which cover the widest range of resource categories. However, these methods do not link exergy consumption to changes in availability or provisioning capacity of a specific natural resource (e.g., mineral, water, land etc.). So far, there is no agreement in the scientific community on the most relevant type of future resource indicators (depletion, increased energy use or cost due to resource extraction, etc.).

To address this challenge, a framework based on the concept of stock/fund/flow resources is proposed to identify, across natural resource categories, whether depletion/dissipation (of stocks and funds) or competition (for flows) is the main relevant aspect.

An LCIA method—or a set of methods—that consistently address all natural resource categories is needed in order to avoid burden shifting from the impact associated with one resource to the impact associated with another resource. This paper is an important basis for a step forward in the direction of consistently integrating the various natural resources as an Area of Protection into LCA.

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USEtox® 2.0 Documentation (Version 1.00)

This document represents the official Documentation of USEtox, the United Nations Environment Programme (UNEP) / Society of Environmental Toxicology and Chemistry (SETAC) scientific consensus model for characterizing human and ecotoxicological impacts of chemical emissions in life cycle assessment. Main output of USEtox is a database of «recommended» and «indicative» characterization factors for human toxicity and freshwater ecotoxicity, based on modelling of environmental fate, exposure, and effect parameters for the substances. Due to deficiencies in the model or the available substance data, the «indicative» factors are accompanied by a higher uncertainty than the «recommended» factors, which should be considered when applying the factors and interpreting the results.


The latest official release version of USEtox is available at http://usetox.org

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A consistent framework for modeling inorganic pesticides: Adaptation of life cycle inventory models to metal-base pesticides

Quantifying over the life cycle of a product or service the chemical emissions to the environment in the life cycle inventory (LCI) phase is typically based on generic assumptions. Regarding the LCI application to agricultural systems the estimation of pesticide emissions is often based on standard emission factors (percentages) or dynamic models based on specific application scenarios that describe only the behavior of organic pesticides. Currently fixed emission fractions for pesticides dearth to account for the influence of pesticide-specific function to crop type and application methods. On the other hand the dynamic models need to account for the variability in this interactions in emissions of inorganic pesticides. This lack of appropriate models to estimate emission fractions of inorganic pesticides results in a lower accuracy when accounting for emissions in agriculture, and it will influence the outcomes of the impact profile. The pesticide emission model PestLCI 2.0 is the most advanced currently available inventory model for LCA intended to provide an estimation of organic pesticide emission fractions to the environment. We use this model as starting point for quantifying emission of inorganic pesticides and customize it taking into account the complex chemistry of metals in order to properly reflect the their environmental fate behavior. We identified specific needs for metal-specific pesticides emission modeling looking at the current PestLCI structure and propose an approach for the different metal-related processes and interactions. The proposed framework takes into consideration the speciation of the metals to accurately describe the soil processes (runoff and leaching). The processes involving degradation are assumed not significant for metals and volatilization is only accounted for special cases (i.e. mercury). And finally, a new module of erosion is included in the modified PestLCI model, because the transport of soil particles to which the metals are bound needs to be considered as potential source of emissions to surface water. In conclusion, we provide a starting point to better estimate metal-specific pesticide emission fractions, addressing the issue of inorganic pesticides for inventory analysis in LCA of agricultural systems.

A flexible matrix-based human exposure assessment framework suitable for LCA and CAA

Humans can be exposed to chemicals via near-field exposure pathways (e.g. through consumer product use) and far-field exposure pathways (e.g. through environmental emissions along product life cycles). Pathways are often complex where chemicals can transfer directly from products to humans during use or exchange between near-and far-field compartments until sub -fractions reach humans via inhalation, ingestion or dermal uptake. Currently, however, multimedia exposure models mainly focus on far-field exposure pathways. Metrics and modeling approaches used in far-field, emission-based models are not applicable to all types of near-field chemical releases from consumer products, e.g. direct dermal application. A consistent near-and far-field framework is needed for life cycle assessment (LCA) and chemical alternative assessment (CAA) to inform mitigation of human exposure to harmful chemicals. To close the current research gaps, we (i) define a near-and far-field matrix-based exposure pathways framework that builds on a quantitative metric based on chemical mass in products, (ii) provide input data for the framework, e.g. chemical concentrations in products linked to functional use categories, and (iii) propose a consistent set of underlying models to populate the matrix-based framework for all relevant multimedia transfers and exposure pathways. Output is a flexible mass balance-based model structuring multimedia transfers in a matrix of first-order inter-compartmental transfer fractions. Inverting this matrix yields cumulative multimedia transfer fractions and exposure pathway-specific Product Intake Fractions defined as chemical mass taken in by humans per unit mass of chemical in a product. When the chemical mass in products is unavailable from individual studies and databases, it can be estimated from chemical-product function relationships or regulatory frame formulations. Combining Product Intake Fractions with chemical masses in products yields exposure estimates per unit mass compatible with LCA and CAA. We demonstrate how this matrix-based modeling system offers a consistent and efficient
way to compare exposure pathways for different user groups (e.g. children and adults) and the general population exposed via the environment associated with product use. Our framework constitutes a user-friendly approach to test and interpret multiple human exposure scenarios in a coupled system of near-and far-field pathways and helps to understand the contribution of individual pathways to overall human exposure in various product application contexts. When combined with toxicity information this approach is a resourceful way to inform LCA and CAA and minimize human exposure to toxic chemicals in consumer products through both product use and environmental emissions.

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A life-cycle assessment of poly-hydroxybutyrate extraction from microbial biomass using dimethylcarbonate
Plastic materials have wide commercial applicability. However, they are made from non-renewable resources and are characterised by resistance to degradation. Poly-hydroxyalkanoates (PHAs) provides one example of a polymer biodegradable, biocompatible and produced from renewable raw materials. With respect to other bioplastics the share of PHAs in the market is very limited because of their commercial costs. To develop more cost effective processes for PHAs production, a multilevel approach is usually undertaken combining innovative, cheaper and more effective cultivation with safe and cheap extraction and purification methodologies. This study assesses the potential environmental impacts related to a production processes based on the novel protocol to extract PHAs comparing them to the impacts of extraction process based on the use of halogenated hydrocarbons.

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Area of Concern: A new paradigm in life cycle assessment for the development of footprint metrics
As a class of environmental metrics, footprints have been poorly defined, have shared an unclear relationship to life cycle assessment (LCA), and the variety of approaches to quantification have sometimes resulted in confusing and contradictory messages in the marketplace. In response, a task force operating under the auspices of the UNEP/SETAC Life Cycle Initiative project on environmental life cycle impact assessment (LCIA) has been working to develop generic guidance for developers of footprint metrics. The purpose of this paper is to introduce a universal footprint definition and related terminology as well as to discuss modelling implications. The task force has worked from the perspective that footprints should be based on LCA methodology, underpinned by the same data systems and models as used in LCA. However, there are important differences in purpose and orientation relative to LCA impact category indicators. Footprints have a primary orientation toward society and nontechnical stakeholders. They are also typically of narrow scope, having the purpose of reporting only in relation to specific topics. In comparison, LCA has a primary orientation toward
stakeholders interested in comprehensive evaluation of overall environmental performance and trade-offs among impact categories. These differences create tension between footprints, the existing LCIA framework based on the area of protection paradigm and the core LCA standards ISO14040/44. In parallel to area of protection, we introduce area of concern as the basis for a universal footprint definition. In the same way that LCA uses impact category indicators to assess impacts that follow a common cause-effect pathway toward areas of protection, footprint metrics address areas of concern. The critical difference is that areas of concern are defined by the interests of stakeholders in society rather than the LCA community. In addition, areas of concern are stand-alone and not necessarily part of a framework intended for comprehensive environmental performance assessment. The area of concern paradigm is needed to support the development of footprints in a way that fulfils their distinctly different purpose. It is also needed as a mechanism to extricate footprints from some of the provisions of ISO 14040/44 which are not considered relevant. Specific issues are identified in relation to double counting, aggregation and the selection of relevant indicators. The universal footprint definition and related terminology introduced in this paper create a foundation that will support the development of footprint metrics in parallel with LCA.
A suggested minimum data list for documenting experimental plant uptake studies

Bio-based chemicals - green, but also sustainable?

For almost two decades, the chemical industry has put great effort into developing bio-chemicals, among others to fight global warming caused by greenhouse gas emissions, one of the biggest threats that are faced by our society today. To facilitate a growing and versatile bio-based chemical production, the US Department of Energy proposed in 2004 a list of 12 building block chemicals which can either be converged through biological or chemical conversions. Moving toward more bio-based chemicals, the chemical industry does not only claim to reduce climate change impacts, but also that they are increasing overall sustainability in chemical production. Whether such claims are justifiable is unclear. When sustainability of bio-based polymer production is assessed, various environmental trade-offs occur that need to be considered. It is not enough to claim that a bio-chemical is sustainable by exclusively looking at reduced global warming impacts related to avoiding oil refining and related greenhouse gas emissions. However, there is big variation of which impacts are assessed and which life cycle stages are included between existing published studies focusing on assessing environmental sustainability of bio-based polymers.
Characterizing health impacts from indoor and outdoor exposure to fine particulates

Exposure to fine particulate matter (PM2.5) pollution is a major contributor to human disease burden as continuously shown in the Global Burden of Disease study series. Exposures to PM2.5 concentration outdoors and indoors contribute almost equally to this burden. Despite the importance, health impacts from exposure to PM2.5 are often excluded from life cycle impact assessment (LCIA) characterization profiles. This is in large part because of the lack of well-vetted harmonized guidance about how to consistently assess the exposures and impacts of indoor and outdoor emissions of PM2.5 and its precursors. We present a framework for calculating characterization factors for indoor and outdoor emissions of primary PM2.5 and secondary PM2.5 precursors, and a roadmap for further refining this modelling framework for operational use in LCIA. The framework was developed over the last three years by a task force convened under SETAC/UNEP auspices.

A recent SETAC Pellston Workshop® was convened to formalize guidance and methods for estimating the health impacts associated with PM2.5 exposure and to recommend PM2.5 characterization factors for application in life cycle assessment. The framework involves three stages—analyzing PM2.5 fate and exposure (including indoor and outdoor urban/rural environments), modeling exposure-response, and the integration of exposure-response and PM2.5 exposure reflecting population and location characteristics. Our exposure model is organized as a mass balance matrix that tracks the global fate of primary PM2.5 and secondary PM2.5 precursor emissions (both indoors and outdoors) as an embedded system of compartments including urban environments, rural environments, and indoor environments within urban and rural areas. After presenting the model structure, we will review initial results and will present geographic variability, discuss key uncertainties, and evaluate our model using results from other models and concentration measurements.

General information
State: Published
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Combined nutritional and environmental life cycle assessment of fruits and vegetables

Nutritional health effects from the ‘use stage’ of the life cycle of food products can be substantial, especially for fruits and vegetables. To assess potential one-serving increases in fruit and vegetable consumption in Europe, we employ the Combined Nutritional and Environmental LCA (CONE-LCA) framework that compares environmental and nutritional effects of foods in a common end-point metric, Disability Adjusted Life Years (DALY). In the assessment, environmental health impact categories include green house gases, particulate matter (PM), and pesticide residues on fruits and vegetables, while for nutrition we consider all health outcomes associated with fruit and vegetable consumption based on epidemiological studies from the global burden of disease (GBD). Findings suggest that one fruit/vegetable serving increase may lead to substantial nutritional health benefits even when considering uncertainty; 35 μDALY/serving fruit benefit compared to a factor 10 lower impact. Replacing detrimental foods, such as trans-fat and red meat, with fruits or vegetables further enhances health benefit. This study illustrates the importance of considering nutritional effects in food-LCA.

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Comprehensive assessment of fruits and vegetables human health effects in a LCA context

Nutritional effects from the 'use stage' of food items life cycle can have a substantial effect on human health; yet, they are often not considered in life cycle assessment (LCA). In our study we explore the case of increased fruit and vegetable consumption, a healthy dietary option – that could result in higher exposures to a wide variety of pesticides – and investigate the trade-offs between associated environmental and nutritional health effects. Methods: We employ the Combined Nutritional and Environmental Life Cycle Assessment (CONE-LCA) framework that evaluates and compares in parallel the environmental and nutritional effects of foods expressed in Disability Adjusted Life Years (DALYs). For the environmental health assessment we consider impact categories such as global warming and particulate matter (PM) as well as chemical exposure due to pesticide residues. Global warming and PM are assessed following a traditional LCA approach. For the pesticide residue exposure, we use publicly available health impact scores derived from toxicological studies of numerous pesticide active ingredients. For the nutritional assessment we focus on the various health outcomes considered in the global burden of disease that are based on epidemiological studies. Results and discussion: Adding one serving of fruits or vegetables to the current average diet in Europe may lead to substantial nutritional health benefits. These nutritional benefits are slightly increased when we consider substitution scenarios in which the substituted food items are associated with negative health effects, such as red meat and trans-fat. Overall environmental health impacts associated with this addition are substantially smaller compared to nutritional benefits in each scenario, even when considering an uncertainty factor of 400 for the impacts of pesticide residues. Conclusion: The present study illustrates the importance of considering nutritional effects of food items in LCA. Our preliminary results suggest that nutritional health effects of food items can be substantial and comparable to environmental impacts, especially for nutritional foods such as fruits and vegetables. This approach could be used for making recommendations about sustainable diets and food choices.

Coupled near-field and far-field exposure assessment framework for chemicals in consumer products

Humans can be exposed to chemicals in consumer products through product use and environmental emissions over the product life cycle. Exposure pathways are often complex, where chemicals can transfer directly from products to humans during use or exchange between various indoor and outdoor compartments until sub-fractions reach humans. To consistently evaluate exposure pathways along product life cycles, a flexible mass balance-based assessment framework is presented structuring multimedia chemical transfers in a matrix of direct inter-compartmental transfer fractions. By matrix inversion, we quantify cumulative multimedia transfer fractions and exposure pathway-specific product intake fractions defined as chemical mass taken in by humans per unit mass of chemical in a product. Combining product intake fractions with chemical mass in the product yields intake estimates for use in life cycle impact assessment and chemical alternatives assessment, or daily intake doses for use in risk-based assessment and high-throughput screening. Two illustrative examples of chemicals used in personal care products and flooring materials demonstrate how this matrix-based framework offers a consistent and efficient way to rapidly compare exposure pathways for adult and child users and for the general population. This framework constitutes a user-friendly approach to develop, compare and interpret multiple
human exposure scenarios in a coupled system of near-field ('user' environment), far-field and human intake compartments, and helps understand the contribution of individual pathways to overall human exposure in various product application contexts to inform decisions in different science-policy fields for which exposure quantification is relevant.

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Estimating pesticide emission fractions for use in LCA: A global consensus-building effort

A practical challenge in LCA for comparing pesticide application in different agricultural practices is the agreement on how to quantify the amount emitted, while only the amount applied to the field is known. Main goal of this paper is to present an international effort carried out to reach agreement on recommended default agricultural pesticide emission fractions to environmental media. Consensual decisions on the assessment framework are (a) primary distributions are used as inputs for LCIA, while further investigating how to assess secondary emissions, (b) framework and LCA application guidelines and documentation will be compiled, (c) the emission framework will be based on modifying PestLCI 2.0, (d) drift values will be provided by German, Dutch and other drift modelers, (e) pesticide application methods will be complemented to develop scenarios for tropical regions, (f) climate, soil and application method scenarios will be based on sensitivity analysis, (g) default emission estimates for LCA will be derived from production-weighted averages, and (h) emission fractions will be reported spatially disaggregated. Recommendations for LCA practitioners and database developers are (a) LCA studies should state whether the agricultural field belongs to technosphere or ecosphere, (b) additional information needs to be reported in LCI (e.g. pesticide mass applied), (c) emissions after primary distribution and secondary fate processes should be reported, (d) LCIA methods should allow for treating the field as part of technosphere and ecosphere, (e) fate and exposure processes should be included in LCIA (e.g. crop uptake), (f) default emission estimates should be used in absence of detailed scenario data, (g) and all assumptions should be reported. The recommended pesticide emission fractions results and recommendations are presented and disseminated to strive for broad acceptance at a dedicated stakeholder workshop back-to-back with the current LCA Food 2016 conference in Dublin.

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Centre de cooperation Internationale en Recherche Agronomique pour le Développement, Life Cycle Strategies, Quantis, IRSTEA ELSA -PACT
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Exposure to chemicals in consumer products: The role of the near-field environment
Humans can be exposed to chemicals in consumer products during product use and environmental releases with inhalation, ingestion, and dermal uptake as typical exposure routes. Nevertheless, chemical exposure modeling has traditionally focused on the far-field with near-field indoor models only recently gaining attention. Further, models that are mostly emissions-based, may not necessarily be applicable to all types of chemical release from consumer products. To address this gap, we (1) define a framework to simultaneously account for exposure to chemicals in the near- and far-field, (2) determine chemical product concentrations for various functional use categories, (3) introduce a quantitative metric linking exposure to chemical mass in products, the Product Intake Fraction (PIF), and (4) demonstrate our framework for various consumer product categories. This framework lends itself to high-throughput calculations for characterizing exposure to the vast consumer product chemical space. The chemical mass in products is used as a starting point for quantifying human exposure obtained by multiplying the chemical concentration (e.g. % w/w) in the product with the amount of product used per defined application. Chemical concentrations in products can be obtained from empirical studies, formulations and associations described in databases, or when unavailable, estimated based on chemical-product functions or regulatory frame formulations. Exposure is quantified by estimating the PIF, the fraction of the chemical in a product that is taken in by humans via each exposure pathway, considering specific compartments of entry into the near-field environment (releases of chemicals encapsulated in articles, indoor air spray, etc.). To estimate PIFs, we combined far-field environmental compartments with near-field compartments and exposure pathways in a multimedia matrix of transfer fractions, with columns and rows for each compartment and exposure pathway. The multiple transfers and PIFs (e.g. from chemicals encapsulated in articles to inhalation of indoor air and dermal uptake via skin contact) were obtained by inverting the transfer fractions matrix, yielding cumulative multimedia transfer fractions. PIFs for various chemicals in products were found to be on the order of 1x10^-7 for semi-volatile organic compounds (SVOCs) in thick flooring, 5x10^-3 for VOCs in indoor air spray, and up to 95% or even higher for ingredients in leave-on cosmetic products.
Exposure to Chemicals in Consumer Products: The Role of the Near-Field Environment

Hazardous chemicals in packaging, including 'eco-friendly' and recycled food packaging, can migrate into food and expose humans. LCA has been fundamental to indicate more 'eco-friendly' packages, but currently LCA does not consider exposure to chemical migrants and methods have not yet been developed. In this study we question if exposure to chemicals in food packaging should be considered as a sustainable design consideration, i.e. if this human health risk is relevant in a life cycle context. To answer this question, we focus on developing methods to quantify exposure to chemicals in food packaging in a life cycle impact assessment (LCIA) framework. To put exposure during use in a life cycle context we perform a screening-level LCA of several life cycle stages of high impact polystyrene packaging (HIPS), with a functional unit of containing and delivering one kilogram of yogurt for consumption. For screening, we include exposure via environmental emissions from the production of the raw material HIPS, thermoforming into packaging, 14 day refrigeration by consumers, and disposal via incineration. The purpose of this screening is not to obtain a detailed and accurate LCA of HIPS but to provide life cycle context to compare the magnitude of characterized exposure to chemicals in packaging, in order to elucidate if this exposure pathway is important. We detail estimates of life cycle exposure to one known hazardous chemical in polystyrene packaging (styrene) that has data available on concentrations in yogurt packaged in HIPS and life cycle inventory releases. We also extend this analysis, given data limitations, to include exposure to three other chemicals in HIPS packaging through food. Given that data on concentrations of food packaging chemicals in food are often missing, we also explore methods to model the product intake fraction (PIF) as the fraction of chemical mass taken in through food packaging versus its initial mass in the food packaging. Results demonstrated that in the given cases consumer exposure to chemicals in packaging through consuming packaged food can be greater than population-level exposure mediated by the life cycle releases of such chemicals, even when only considering one or several chemicals in packaging that expose consumers. Occupational exposure was not considered in this study, but could be a focus of future work. Thus, this initial exploration indicates that exposure to chemicals in food packaging can be an essential consideration for burden shifting and quantifying design trade-offs in a life cycle context.
Framework for Multi-Pathway Cumulative Exposure for Comparative Assessments

Efforts to assess human and ecosystem exposure to contaminants released to multiple environmental media have been evolving over the last decades. In this talk, we summarize the development and evolution of the multimedia mass-balance approach combined with multi-pathway exposure assessment as a framework for comparative assessment of chemicals, products, and services. We first review the development and evolution of the multimedia mass-balance approach to pollutant fate and exposure evaluation and illustrate some of the calculations used in multimedia, multi-pathway exposure assessments. The multimedia approach requires comprehensive assessments that locate all points of chemical release to the environment, characterize mass-balance relationships, and track contaminants through the entire environmental system to exposure of individuals or populations or specific ecosystems. For use in comparative risk assessment, life-cycle assessment (LCA), and chemical alternatives assessment (CAA), multimedia fate and exposure models synthesize information about partitioning, reaction, and intermedia-transport properties of chemicals in a representative (local to regional) or generic (continental to global) environment with information about larger scale populations rather than specific individuals or vulnerable subgroups. Although there can be large uncertainties in this approach, it provides insight on how chemical properties and use patterns map onto population-scale metrics of exposure, such as intake fraction for characterizing human intake per unit emission and aquatic or terrestrial ecosystem exposure concentrations per unit emission. We next discuss the reliability with which fate models at different levels of geographic scale—from near field indoor scales to urban, regional, continental and even global scale—can be used to determine cumulative human exposure and/or ecosystem exposure from multiple pollutants and emissions sources. The key question here is whether the results of cumulative assessments can provide sufficient insight for decision makers who are concerned with life-cycle impacts and chemical alternatives. We present a regional case study for pesticide alternatives in an agricultural valley of California to assess the opportunities and future prospects for the multi-pathway cumulative framework in LCA and CAA. This case reveals that the relative contributions to cumulative pollutant intake via different exposure pathways depend on (a) persistence of chemicals at different levels of integration (regional, urban-scale, food-web, indoors), (b) basic chemical properties, (c) the retention of chemicals in food webs, and (d) the retention of chemicals by indoor surfaces.

Getting the chemicals right: addressing inorganics in sustainability assessments of technologies

A main goal of sustainability research is to enable a technological development in industry and elsewhere that ensures that what is produced and how it is produced today does not harm the quality of human or environmental health for present and future generations. As part of current environmental sustainability assessments, the toxicity potential of several thousand organic chemicals
is included in characterization models within life cycle impact assessment (LCIA). However, many economic production processes involve the use of inorganic chemicals to a large extent, while the related pressure on human and environmental health of environmental emissions of these substances is not yet fully understood and not included in any existing LCIA method. In this presentation, we provide an overview of the relevance of inorganic chemicals and outline possible ways towards incorporating inorganic chemicals in LCIA toxicity characterization.

Global guidance on environmental life cycle impact assessment indicators: Progress and case study

Purpose
The life cycle impact assessment (LCIA) guidance flagship project of the United Nations Environment Programme (UNEP)/Society of Environmental Toxicology and Chemistry (SETAC) Life Cycle Initiative aims at providing global guidance and building scientific consensus on environmental LCIA indicators. This paper presents the progress made since 2013, preliminary results obtained for each impact category and the description of a rice life cycle assessment (LCA) case study designed to test and compare LCIA indicators.

Methods
The effort has been focused in a first stage on impacts of global warming, fine particulate matter emissions, water use and land use, plus cross-cutting issues and LCAbased footprints. The paper reports the process and progress and specific results obtained in the different task forces (TFs). Additionally, a rice LCA case study common to all TF has been developed. Three distinctly different scenarios of producing and cooking rice have been defined and underlined with life cycle inventory data. These LCAs help testing impact category indicators which are being developed and/or selected in the harmonisation process. The rice LCA case study further helps to ensure the practicality of the finally recommended impact category indicators.

Results and discussion
The global warming TF concludes that analysts should explore the sensitivity of LCA results to metrics other than GWP. The particulate matter TF attained initial guidance of how to include health effects from PM$_{2.5}$ exposures consistently into LCIA. The biodiversity impacts of land use TF suggests to consider complementary metrics besides species richness for assessing biodiversity loss. The water use TF is evaluating two stress-based metrics, AWARe and an alternative indicator by a stakeholder consultation. The cross-cutting issues TF agreed upon maintaining disability-adjusted life years (DALY) as endpoint unit for the safeguard subject "human health". The footprint TF defined main attributes that should characterise all footprint indicators. "Rice cultivation" and "cooking" stages of the rice LCA case study contribute most to the environmental impacts assessed.

Conclusions
The results of the TF will be documented in white papers and some published in scientific journals. These white papers represent the input for the Pellston workshop ™, taking place in Valencia, Spain, from 24 to 29 January 2016, where best practice, harmonised LCIA indicators and an update on the general LCIA framework will be discussed and agreed on. With the diversity in results and the multi-tier supply chains, the rice LCA case study is well suited to test candidate recommended indicators and to ensure their applicability in common LCA case studies.
We aim to develop harmonized and operational methods for quantifying exposure to chemicals in food packaging specifically for sustainability assessments. Thousands of chemicals are approved for food packaging and numerous contaminants occur, e.g., through recycling. Chemical migration into food, as a function of the chemical, food, and package properties and storage conditions, is responsible for human exposure to many chemicals of concern. In addition to complying with regulatory standards, stakeholders concerned with environmental sustainability draw on strategies such as Life Cycle Assessment (LCA) and Cradle to Cradle to support packaging design. Each assessment has distinct context and goals, but can help manage exposure to toxic chemicals and other environmental impacts. Metrics and methods to quantify and characterize exposure to potentially toxic chemicals specifically in food packaging are, however, notably lacking from such assessments. Furthermore, previous case studies demonstrated that sustainable packaging design focuses, such as decreasing greenhouse gas emissions or resource consumption, can increase exposure to toxic chemicals through packaging. Thereby, developing harmonized methods for quantifying exposure to chemicals in food packaging is critical to ensure ‘sustainable packages’ do not increase exposure to toxic chemicals. Therefore we developed modelling methods suitable for first-tier risk screening and environmental assessments. The modelling framework was based on the new product intake fraction (PiF) exposure metric, with units of chemical mass taken in by exposed persons versus chemical mass within a product. To model this metric, we used analytical approximations for regulatory models. We
investigated model results for various chemical -package-food combinations to facilitate operation in assessments and identify combinations of priority. Modelling results predicted with accuracy previous findings, that exposure is dependent on diffusive and partitioning behaviors according to each chemical-package-food combination. Harmonizing exposure modeling with environmental assessments, like LCA, finally facilitates including exposure to chemicals as a sustainable packaging design issue. Results were demonstrated in context of the pilot-scale Product Environmental Footprint regulatory method in the European Union. Increasing recycled content, decreasing greenhouse gas emissions by selecting plastics over glass, and adding chemicals with a design function were identified as risk management issues. We conclude developing an exposure framework, suitable for sustainability assessments commonly used for food packaging, is feasible to help guide packaging design to consider both the environment and human exposure. Future work is required for refinement and operationality. This is the first study addressing the need for quantitative, harmonized exposure metrics and methods for food packaging within sustainability assessment frameworks.

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Health effects from indoor and outdoor exposure to fine particulate matter in life cycle impact assessment
Fine particulate matter (PM2.5) pollution has been estimated to contribute more than 7% to the total global human disease burden from 1990 to 2013 (http://healthdata.org/gbd). Ambient (outdoor) and household indoor PM2.5 exposures are reported to account for 41% and 58% of this impact, respectively, emphasizing the need to include both, outdoor and indoor exposure into overall estimates of health burdens in life cycle impact assessment. However, lacking clear guidance on how to consistently include health effects from exposure to PM2.5 in life cycle perspective, practitioners fail to report related life cycle impacts. To address this gap, a global initiative has worked on building a coupled indoor-outdoor intake fraction framework combining exposure to PM2.5 emitted indoors and outdoors with exposure to PM2.5 formed indoors and outdoors from chemical reactions. An exposure-response model derived from ambient PM2.5 concentrations is consistently combined with exposures from indoor and outdoor sources. All factors are systematically built into a model parameterized for different archetypal outdoor and indoor settings, such as specific residential and occupational settings and different urban area sizes. Model and parameters are tested in a case study on the production and processing of rice in three distinct scenarios covering urban China, rural India and U.S.-Europe. Recommendations are to use this coupled, generic framework whenever emission locations are unknown and to apply spatial models whenever emission locations are known. Our study constitutes a first step towards providing guidance on how to include health effects from PM2.5 indoor air exposures in product-oriented impact assessments.

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Health effects from indoor and outdoor exposure to fine particulate matter in life cycle impact assessment

Exposure to fine particulate matter (PM2.5) pollution is a major contributor to human disease burden as continuously shown in the Global Burden of Disease study series. Exposures to PM2.5 concentration outdoors and indoors contribute almost equally to this burden. Despite the importance, health impacts from exposure to PM2.5 are often excluded from life cycle impact assessment (LCIA) characterization profiles. This is in large part because of the lack of well-vetted harmonized guidance about how to consistently assess the exposures and impacts of indoor and outdoor emissions of PM2.5 and its precursors. We present a framework for calculating characterization factors for indoor and outdoor emissions of primary PM2.5 and secondary PM2.5 precursors, and a roadmap for further refining this modelling framework for operational use in LCIA. The framework was developed over the last three years by a task force convened under SETAC/UNEP auspices and culminating in a recent international expert workshop, to provide guidance and methods for estimating the health impacts associated with PM2.5 exposure and to recommend PM2.5 characterization factors for application in life cycle assessment. The framework involves three stages – analyzing PM2.5 fate and exposure (including indoor and outdoor urban/rural environments), modeling exposure-response, and the integration of exposure-response and PM2.5 exposure reflecting population and location characteristics. Our exposure model is organized as a mass balance matrix that tracks the global fate of primary PM2.5 and secondary PM2.5 precursor emissions (both indoors and outdoors) as an embedded system of compartments including urban environments, rural environments, and indoor environments within urban and rural areas. After presenting the model structure, we will review initial results and will present geographic variability, discuss key uncertainties, and evaluate our model using results from other models and concentration measurements.

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Health impacts of fine particulate matter

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HESI pilot project: Testing a qualitative approach for incorporating exposure into alternatives assessment

Most alternatives assessments (AA) published to date are largely hazard-based rankings, and as such may not serve to determine a practical and functional replacement. With an assessment goal of identifying an alternative chemical that is more sustainable, other attributes beyond hazard are also important, including exposure, risk, life-cycle thinking, performance, cost, and social responsibility. Building on the 2014 recommendations by the US National Academy of Sciences to improve AA decisions by including comparative exposure assessment, the HESI Sustainable Chemical Alternatives Technical Committee, which consists of scientists from academia, industry, government, and NGOs, has developed a qualitative comparative exposure approach. Conducting such a comparison can screen for
alternatives that are expected to have a higher exposure potential, which could trigger a higher-tiered, more-quantitative exposure assessment on the alternatives being considered.

This talk will demonstrate an approach for including chemical and product exposure information in a qualitative AA comparison. Starting from existing hazard AAs, a series of four exposure examples were examined to test the concept, to understand the effort required, and to determine the value of exposure data in AA decision-making. The group has developed ingredient and product parameter categorization to support comparisons between chemicals and methodology to address data quality. The ingredient parameters include a range of physicochemical properties that can impact exposure, while the product parameters include aspects such as exposure pathway, use pattern, frequency/duration of use, concentration in product and use volume, accessibility, and disposal. Key learnings, challenges, and opportunities for further work will also be presented.

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High-throughput exposure modeling to support prioritization of chemicals in personal care products

We demonstrate the application of a high-throughput modeling framework to estimate exposure to chemicals used in personal care products (PCPs). As a basis for estimating exposure, we use the product intake fraction (PiF), defined as the mass of chemical taken by an individual or population per mass of a given chemical used in a product. We calculated use- and disposal- stage PiFs for 518 chemicals for five PCP archetypes. Across all product archetypes the use- and disposal- stage PiFs ranged from 10−5 to 1 and 0 to 10−3, respectively. There is a distinction between the use-stage PiF for leave-on and wash-off products which had median PiFs of 0.5 and 0.02 across the 518 chemicals, respectively. The PiF is a function of product characteristics and physico-chemical properties and is maximized when skin permeability is high and volatility is low such that there is no competition between skin and air losses from the applied product. PCP chemical contents (i.e. concentrations) were available for 325 chemicals and were combined with PCP usage characteristics and PiF yielding intakes summed across a demonstrative set of products ranging from 10−8–30 mg/kg/d, with a median of 0.1 mg/kg/d. The highest intakes were associated with body lotion. Bioactive doses derived from high-throughput in vitro toxicity data were combined with the estimated PiFs to demonstrate an approach to estimate bioactive equivalent chemical content and to screen chemicals for risk.

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Impacts of food consumption: A missing hot spot in LCA?

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Improving plant bioaccumulation science through consistent reporting of experimental data
Experimental data and models for plant bioaccumulation of organic contaminants play a crucial role for assessing the potential human and ecological risks associated with chemical use. Plants are receptor organisms and direct or indirect vectors for chemical exposures to all other organisms. As new experimental data are generated they are used to improve our understanding of plant-chemical interactions that in turn allows for the development of better scientific knowledge and conceptual and predictive models. The interrelationship between experimental data and model development is an ongoing, never-ending process needed to advance our ability to provide reliable quality information that can be used in various contexts including regulatory risk assessment. However, relatively few standard experimental protocols for generating plant bioaccumulation data are currently available and because of inconsistent data collection and reporting requirements, the information generated is often less useful than it could be for direct applications in chemical assessments and for model development and refinement. We review existing testing guidelines, common data reporting practices, and provide recommendations for revising testing guidelines and reporting requirements to improve bioaccumulation knowledge and models. This analysis provides a list of experimental parameters that will help to develop
high quality datasets and support modeling tools for assessing bioaccumulation of organic chemicals in plants and ultimately addressing uncertainty in ecological and human health risk assessments.

**General information**

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**Organisations:** Department of Management Engineering, Quantitative Sustainability Assessment, ARC Arnot Research and Consulting, Utah State University

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Indoor inhalation intake fractions of fine particulate matter: Review of influencing factors

Exposure to fine particulate matter (PM2.5) is a major contributor to the global human disease burden. The indoor environment is of particular importance when considering the health effects associated with PM2.5 exposures because people spend the majority of their time indoors and PM2.5 exposures per unit mass emitted indoors are two to three orders of magnitude larger than exposures to outdoor emissions. Variability in indoor PM2.5 intake fraction (iFin, total), which is defined as the integrated cumulative intake of PM2.5 per unit of emission, is driven by a combination of building-specific, human-specific, and pollutant-specific factors. Due to a limited availability of data characterizing these factors, however, indoor emissions and intake of PM2.5 are not commonly considered when evaluating the environmental performance of product life cycles. With the aim of addressing this barrier, a literature review was conducted and data characterizing factors influencing iFin, total were compiled. In addition to providing data for the calculation of iFin, total in various indoor environments and for a range geographic regions, this paper discusses remaining limitations to the incorporation of PM2.5-derived health impacts into life cycle assessments and makes recommendations regarding future research.

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Integrated approach for characterizing and comparing exposure-based impacts with life cycle impacts

To address hazardous chemicals in consumer products, chemical alternatives assessment (CAA) is an emerging approach combining hazard and exposure assessment with technical and economic feasibility. Life cycle aspects are typically not consistently considered in CAA, but are relevant to avoid decisions that involve burden shifting or that result in only incremental improvement. Focusing in the life cycle impacts on widely accepted and applied impact categories like global warming potential or cumulative energy demand aggregating several impact categories will lead to underestimations of life cycle emissions of potentially harmful chemicals and their proposed replacements. Hence, an assessment framework is required that is able to account for near-field consumer exposure to chemicals in products during and after product use as well as population far-field exposure to chemical emissions to the environment from product-related processes along the product life cycle. We build on a flexible mass balance-based modeling system yielding cumulative multimedia transfer fractions and exposure pathway-specific Product Intake Fractions defined as chemical mass taken in by humans per unit mass of chemical in a product. When combined chemical masses in products and further with toxicity information, this approach is a resourceful way to inform CAA and minimize human exposure to toxic chemicals in consumer products through both product use and environmental emissions. We use an example of chemicals in consumer products to demonstrate how this matrix-based system offers a consistent and efficient way to compare exposure pathways for different user groups (e.g. children and adults) and the general population exposed via the environment. We further compare toxicity-related outcomes with outcomes from other life cycle impacts to compare the relevance of different impact categories for different consumer product classes. Through our examples, we will show (a) how to align assumptions used in different assessment methods in a manner that can avoid contradictory results, (b) to consistently consider and compare all relevant impacts, thereby avoiding burden shifting that could result from disregarding chemical and product life cycles, and (c) to prioritize the most relevant impacts across all life cycle stages, thereby setting the scene for a “life cycle alternatives assessment” (LCAA).

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Integrated indoor and outdoor exposure assessment framework for fine particulate matter pollution

The 2010 Global Burden of Disease report demonstrates that fine particulate matter (PM2.5) pollution is the major environmental contributor to mortality. Exposures outdoors (ambient) and indoors (household) contribute almost equally to this burden. Unfortunately, the health impacts from exposure to PM2.5 are often excluded from life cycle impact assessment (LCIA) used for characterizing environmental performance of products and services. This is in large part because of the lack of well-vetted harmonized guidance about how to consistently assess the exposures and impacts of indoor and outdoor emissions of PM2.5 and its precursors. We present a modeling framework for calculating exposure factors for indoor and outdoor emissions of primary PM2.5 and secondary PM2.5 precursors, and a roadmap for further refining this modelling framework for operational use in LCIA. The framework was developed over the last three years by a task force convened under auspices of the Society of Environmental Toxicology and Chemistry (SETAC)/United Nations Environment Program (UNEP) Life-Cycle Initiative to provide guidance and methods for estimating the health impacts associated with PM2.5 exposure and to recommend PM2.5 characterization factors for application in life cycle assessment. The framework involves three stages—analyzing PM2.5 fate and exposure (including indoor and outdoor urban/rural environments), modeling exposure-response, and the integration of exposure-response and PM2.5 exposure reflecting population and location characteristics. We introduce the overall framework and present key components of the exposure assessment underlying the health impact characterization factors. The exposure metric at the center of this analysis is the population intake fraction (iF). Our exposure model is organized as a mass balance matrix that tracks the global fate of primary PM2.5 and secondary PM2.5 precursor emissions (both indoors and outdoors) as an embedded system of compartments including urban environments, rural environments, and indoor environments within urban and rural areas. The fate modeling system provides PM2.5 concentrations that are linked with human activity patterns and population geographical distribution patterns to determine intake fractions. After presenting the model structure, we will review initial results and will present geographic variability, discuss key uncertainties, and evaluate our model using results from other models and
Integrating exposure into chemical alternatives assessment using a qualitative approach

Most alternatives assessments (AA) published to date are largely hazard-based rankings, and as such may not represent a fully informed consideration of the advantages and disadvantages of possible alternatives. With an assessment goal of identifying an alternative chemical that is more sustainable, other attributes beyond hazard are also important, including exposure, risk, life-cycle impacts, performance, cost, and social responsibility. Building on the 2014 recommendations by the U.S. National Academy of Sciences to improve AA decisions by including comparative exposure assessment, the HESI Sustainable Chemical Alternatives Technical Committee, which consists of scientists from academia, industry, government, and NGOs, has developed a qualitative comparative exposure approach. Conducting such a comparison can screen for alternatives that are expected to have a higher exposure potential, which could trigger a higher-tiered, more quantitative exposure assessment on the alternatives being considered. This talk will demonstrate an approach for including chemical- and product-related exposure information in a qualitative AA comparison. Starting from existing hazard AAs, a series of four chemical-product application scenarios were examined to test the concept, to understand the effort required, and to determine the value of exposure data in AA decision-making. The group has developed a classification approach for ingredient and product parameters to support comparisons between alternatives as well as methodology to address data quality. The ingredient parameters include a range of physicochemical properties that can impact routes and magnitude of exposure, while the product parameters include aspects such as exposure pathways, use pattern, frequency/duration of use, chemical concentration in product, and use volume, accessibility, and disposal. Key learnings, challenges, and opportunities for further work will also be presented. The views expressed in this presentation do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.
Integrating exposure into chemical alternatives assessment using a qualitative approach

Most alternatives assessments (AA) published to date are largely hazard-based rankings, and as such may not represent a fully informed consideration of the advantages and disadvantages of possible alternatives. With an assessment goal of identifying an alternative chemical that is more sustainable, other attributes beyond hazard are also important, including exposure, risk, life-cycle impacts, performance, cost, and social responsibility. Building on the 2014 recommendations by the U.S. National Academy of Sciences to improve AA decisions by including comparative exposure assessment, the HESI Sustainable Chemical Alternatives Technical Committee, which consists of scientists from academia, industry, government, and NGOs, has developed a qualitative comparative exposure approach. Conducting such a comparison can screen for alternatives that are expected to have a higher human or environmental exposure potential, which could trigger a higher-tiered, more quantitative exposure assessment on the alternatives being considered, minimizing the likelihood of regrettable substitution. This talk will demonstrate an approach for including chemical- and product-related exposure information in a qualitative AA comparison. Starting from existing hazard AAs, a series of three chemical-product application scenarios were examined to test the concept, to understand the effort required, and to determine the value of exposure data in AA decision-making. The group has developed a classification approach for ingredient and product parameters to support comparisons between alternatives as well as methodology to address exposure parameter relevance and data quality. The ingredient parameters include a range of physicochemical properties that can impact routes and magnitude of exposure, while the product parameters include aspects such as exposure pathways, use pattern, frequency/duration of use, chemical concentration in product, and use volume, accessibility, and disposal. Key learnings, challenges, and opportunities for further work will also be presented. The views expressed in this presentation do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.

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Life cycle human health impacts of 875 pesticides

Purpose

Residues in field crops grown and harvested for human consumption are the main contributor to overall human exposure toward agricultural pesticides for the general population. However, exposure from crop residues is currently not considered in life cycle assessment practice. We therefore present a consistent framework for characterizing human toxicological impacts associated with pesticides applied to agricultural crops in the frame of life cycle impact assessment based on state-of-the-art data and methods.

Methods

We combine a dynamic multicrop plant uptake model designed for evaluating human exposure to residues for a wide range of pesticide-crop combinations with latest findings of pesticide dissipation kinetics in crops and post-harvest food processing. Outcome is a set of intake fractions and characterization factors for 875 organic pesticides and six major food crops along with specific confidence intervals for each factor.

Results and discussion

Intake fractions aggregating exposure via crop residues and exposure via fractions lost to air and soil for pesticides applied to agricultural crops vary between 10−8 and 10−1 kg intake per kilogram applied as a function of pesticide and crop. Intake fractions are typically highest for lettuce and tomato and lowest for potato due to differences in application times before crop harvest and soil as additional barrier for uptake into potato tubers. Uncertainty in intake fractions is mainly associated with dissipation dynamics in crops, where results demonstrate that using pesticide- and crop-specific data is crucial. Combined with the uncertainty in effect modeling, characterization factors per pesticide and crop show squared geometric mean standard deviations ranging from 38 to 15,560 over a variability range across pesticide-crop combinations of 10 orders of magnitude.

Conclusions
Our framework is operational for use in current life cycle impact assessment models, is made available for USEtox, and closes an important gap in the assessment of human exposure to pesticides. For ready use in life cycle assessment studies, we present pesticide-crop combination-specific characterization factors normalized to pesticide mass applied and provide default data for application times and loss due to post-harvest food processing. When using our data, we emphasize the need to consult current pesticide regulation, since each pesticide is registered for use on certain crops only, which varies between countries.
Mainstreaming life cycle thinking through a consistent approach to footprints

Over recent years, footprints have emerged as an important means of reporting environmental performance. Some individual footprints have become quite sophisticated in their calculation procedures. However, as an overall class of environmental metrics they have been poorly defined, having a variety of conceptual foundations and an unclear relationship to LCA. The variety and sometimes contradictory approaches to quantification have also led to confusing and contradictory messages in the marketplace which have undermined their acceptance by industry and governments. In response, a task force operating under the auspices of the UNEP/SETAC Life Cycle Initiative project on environmental Life Cycle Impact Assessment has been working to develop generic guidance for developers of footprint metrics. The initial work involved forming a consensual position on the difference between footprints and existing LCA impact category indicators.

In short, footprints are deemed to have a primary orientation toward society and nontechnical stakeholders and report only on selected topics of concern. On the other hand, LCA impact category indicators have a primary orientation toward technical stakeholders and report in relation to a larger framework designed for comprehensive evaluation of environmental performance and trade-offs. The task force has also developed a universal footprint definition. In parallel to Area of Protection, we introduce Area of Concern. In the same way that LCA uses impact category indicators to assess impacts that follow a common cause-effect pathway toward Areas of rotection, footprint metrics address Areas of Concern. The critical difference is that Areas of Concern are defined by the interests of stakeholders in society rather than the LCA community. In addition, Areas of Concern are stand-alone and not part of a framework intended for comprehensive environmental performance assessment. Accordingly, footprints are universally defined as metrics used to report life cycle assessment results addressing an Area of Concern.

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Multi-pathway exposure modelling of chemicals in cosmetics with application to shampoo

We present a novel multi-pathway, mass balance based, fate and exposure model compatible with life cycle and high-throughput screening assessments of chemicals in cosmetic products. The exposures through product use as well as post-use emissions and environmental media were quantified based on the chemical mass originally applied via a product, multiplied by the product intake fractions (PiF, the fraction of a chemical in a product that is taken in by exposed persons) to yield intake rates. The average PiFs for the evaluated chemicals in shampoo ranged from 3 × 10−4 up to 0.3 for rapidly absorbed ingredients. Average intake rates ranged between nano- and micrograms per kilogram bodyweight per day; the order of chemical prioritization was strongly affected by the ingredient concentration in shampoo. Dermal intake and inhalation (for 20% of the evaluated chemicals) during use dominated exposure, while the skin permeation coefficient dominated the estimated uncertainties. The fraction of chemical taken in by a shampoo user often exceeded, by orders of magnitude, the aggregated fraction taken in by the population through post-use environmental emissions. Chemicals with relatively high octanol-water partitioning and/or volatility, and low molecular weight tended to have higher use stage exposure. Chemicals with low intakes during use (< 1%) and subsequent high post-use emissions, however, may yield comparable intake for a member of the general population. The presented PiF based framework offers a novel and critical advancement for life cycle assessments and high-throughput exposure screening of chemicals in cosmetic products demonstrating the importance of consistent consideration of near- and far-field multi-pathway exposures.

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Natural resources as an area of protection in LCA - outcomes of the discussion by the working group on resources within the UNEP-SETAC Life Cycle Initiative

The topic of resources as an area of protection (AoP) in life cycle assessment (LCA) is being discussed within an expert group under the umbrella of the Life Cycle Initiative by the United Nations Environment Programme (UNEP) and the Society for Environmental Toxicology and Chemistry (SETAC). The AoP ‘Natural Resources’ is neither well defined nor agreed upon. Furthermore, there is currently no life cycle impact assessment (LCIA) method available that is able to consistently assess impacts at midpoint and endpoint level across different...
resource categories (minerals/metals and fossil fuels, water, land/soil, biotic resources like wild plants and animals). Definitions and categorizations of natural resources differ and there is no agreement on what methods should be considered midpoint or endpoint methods because there is no agreement (at midpoint and endpoint) on what impact should be assessed (is it reduced availability, is it depletion, is it increased energy use or costs due to future resource extraction, etc.?). The merit of this working group is the broad analysis of available methods considering different resources and their integrated discussion according to the methods’ underlying principles (e.g. use-to-availability ratios, backup technology approaches, etc.). This is the basis on which recommendations for best practice with existing methods and indications for further research and development will be given. At the time of the SETAC 2016 conference, the group should have these recommendations ready.

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Safe and Sustainable: Optimizing Material Flows in a Circular Economy
Increasing the sustainability of a globally connected economy is gaining wide attention in a world with limited natural resources and growing chemical pollution. The circular economy has emerged as away to reduce carbon and other emissions, while increasing resource efficiency over several product life cycles. However, a circular economy is only viable if it is both safe and sustainable. The dilemma is that sustainable does not necessarily imply safe and vice versa. When minimizing exposure to harmful chemicals in consumer products (safe), we often use more energy-demanding alternative solutions (unsustainable). When maximizing resource use efficiency and reducing carbon and other emissions through recycling (sustainable), direct consumer exposure is often increased through cross-contamination of recycled materials (unsafe). Hence, circular economy currently fails to unite the required expertise to simultaneously increase sustainability and reduce exposure to chemicals in materials reused across life cycles of different products. For a way out of this dilemma, a paradigm shift is needed towards a comprehensive and quantitative assessment framework.

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The substitution of hazardous chemicals in the international context - Opportunity for promoting sustainable chemistry
While a wide range of sustainable/green chemicals for various applications is available, often only certain types of hazardous or unsustainably produced chemicals are continued to be used out of different reasons (“lock-in problem”) 1,2. One challenge is that policy makers and industries in particular in developing and transition countries do not know about more sustainable and green alternatives for a chemical in a particular application. Methodologies and tools are, hence, needed for the communication and dissemination of information on more sustainable alternatives. The substitution and phase-out of hazardous chemicals, such as persistent organic pollutants (POPs), on international level like under the Stockholm Convention, might provide one promising mechanism to mainstream more sustainable and greener chemicals and other alternative solutions aiming at eliminating or at least significantly reducing hazardous chemicals in products and other uses. Within the Stockholm Convention - ratified by 179 countries - the POPs Reviewing Committee is evaluating alternatives to POPs and has developed guidance on alternatives assessment. Within the Stockholm Convention activities
on POPs-Phase-Out a publication has been developed compiling information on POPs-phase out and alternatives. In the conclusions and recommendation of this document “Sustainable and Green Chemistry” is highlighted as a guiding principle for alternatives assessment. This could be an entry point of Sustainable Chemistry in the alternatives assessment process on international level. The POPs phase out document links also to the web-platform SUBSPORT (www.subsport.eu) which has been developed in the frame of an EU project for safer alternatives to toxic chemicals. In this presentation the Stockholm Convention alternatives assessment activities and also the SUBSPORT platform are shortly introduced as tools which can be utilized for promoting the use of more sustainable/green chemicals at international level including developing countries.

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**What are the elements required to improve exposure estimates in life cycle assessments?**

In this study we aim to identify and discuss priority elements required to improve exposure estimates in Life cycle assessment (LCA). LCA aims at guiding decision-support to minimize damages on resources, humans, and ecosystems which incur via providing society with products and services. Potential human toxicity and ecosystem toxicity of chemicals posed by different product life cycle stages are characterized in the life cycle impact assessment (LCIA) phase. Exposure and effect quantification as part of LCIA toxicity characterization faces numerous challenges related to inventory analysis (e.g. number and quantity of chemicals emitted), substance-specific modelling (e.g. organics, inorganics, nano-materials) in various environments and time horizons, human and ecosystem exposure quantification (e.g. exposed organisms and exposure pathways), and toxicity end-points (e.g. carcinogenicity). There are many relevant areas for improving exposure quantification in LCIA. We explore prioritising future work based on investigating existing mitigation efforts, observed damages, and potential for (irreversible) harm to ensure LCIA covers at least the most relevant concerns faced by societies today regarding chemical exposure and harmful effects. Thereby, we structure this study of key elements identified as areas of elevated public, industrial, regulatory, and scientific concerns. We found the majority of missing elements are directly related to the definition of exposed populations (both ecosystems and humans). For example, current LCIA human toxicity methods focus on exposure of the general population via chemical emissions. Occupational and consumer exposure to chemicals is of elevated concern for various stakeholders and leads to millions, if not billions, of dollars of damages yearly (e.g. through mesothelioma). Although consumer and occupational exposures often occur at magnitudes far greater than exposure mediated via environmental emissions, they are notably missing from current LCIA methods. As another example, recommended LCIA ecotoxicity methods focus on freshwater ecosystems. A significant amount of resources has been spent to mitigate damages on marine and terrestrial organisms such as fishes, bees, and birds. However, recommended methods are currently unavailable in LCIA to consider these organisms to evaluate the sensitivity of terrestrial and marine ecosystems. Microbes are another elevated concern due to the rise of antibiotic resistant organisms due to microbial exposure to disinfectants, antimicrobials and antibiotics etc. Yet, both the microbial exposure to chemicals and human exposure to microbes (and other disease vectors) are entirely missing from current LCIA exposure frameworks. In all, defining exposure sub-populations and developing suitable methods can improve exposure methods in LCIA and capture major societal concerns.

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Active Learning in Sustainability Teaching

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Office for Study Programmes and Student Affairs
Authors: Laurent, A. (Intern), Olsen, S. I. (Intern), Fantke, P. (Intern), Andersson, P. H. (Intern)
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Aiding Designers to make Practitioner-like Interpretations of Life Cycle Assessment Results

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Indian Institute of Science
Authors: Uchil, P. (Ekstern), Chakrabarti, A. (Ekstern), Fantke, P. (Intern)
Number of pages: 1
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Host publication information
Title of host publication: Programme and Abstract Book. The 20th International Conference on Engineering Design (ICED 2015)
Publisher: Design Society
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Abstract
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A multi-compartmental framework for near and far-field exposure to consumer products

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Fantke, P. (Intern), Ernstoff, A. (Intern), Huang, L. (Ekstern), Csiszar, S. A. (Ekstern), Jolliet, O. (Ekstern)
Pages: 74-75
Publication date: 2015

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Title of host publication: Abstract Book. ISES 25th Annual Meeting : Exposures in an Evolving Environment
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A_multi_compartmental_framework.pdf
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Analysing half-lives for pesticide dissipation in plants
Overall dissipation of pesticides from plants is frequently measured, but the contribution of individual loss processes is largely unknown. We use a pesticide fate model for the quantification of dissipation by processes other than degradation. The model was parameterised using field studies. Scenarios were established for Copenhagen/Denmark and Shanghai/PR China, and calibrated with measured results. The simulated dissipation rates of 42 pesticides were then compared with measured overall dissipation from field studies using tomato and wheat. The difference between measured overall dissipation and calculated dissipation by non-degradative processes should ideally be contributable to degradation in plants. In 11% of the cases, calculated dissipation was above the measured dissipation. For the remaining cases, the non-explained dissipation ranged from 30% to 83%, depending on crop type, plant part and scenario. Accordingly, degradation is the most relevant dissipation process for these 42 pesticides, followed by growth dilution. Volatilisation was less relevant, which can be explained by the design of plant protection agents. Uptake of active compound from soil into plants leads to a negative dissipation process (i.e. a gain) that is difficult to quantify because it depends largely on interception, precipitation and plant stage. This process is particularly relevant for soluble compounds.

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Department of Environmental Engineering, Environmental Chemistry, Technical University of Denmark
Authors: Jacobsen, R. (Ekstern), Fantke, P. (Intern), Trapp, S. (Intern)
Pages: 325–342
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Scopus rating (2015): SJR 0.473 SNIP 0.748
BFI (2014): BFI-level 1
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Assessing comparative terrestrial ecotoxicity of Cd, Co, Cu, Ni, Pb, and Zn: The influence of aging and emission source

Metal exposure to terrestrial organisms is influenced by the reactivity of the solid-phase metal pool. This reactivity is thought to depend on the type of emission source, on aging mechanisms that are active in the soil, and on ambient conditions. Our work shows, that when controlling for soil pH or soil organic carbon, emission source occasionally has an effect on reactivity of Cd, Co, Cu, Ni, Pb and Zn emitted from various anthropogenic sources followed by aging in the soil from a few years to two centuries. The uncertainties in estimating the age prevent definitive conclusions about the influence of aging time on the reactivity of metals from anthropogenic sources in soils. Thus, for calculating comparative toxicity potentials of man-made metal contaminations in soils, we recommend using time-horizon independent accessibility factors derived from source-specific reactive fractions.
Comparative exposure to DEHP from food contact materials: application of the product intake fraction

Quantitative Sustainability Assessment Food contact materials (FCM), e.g., bottles and food handling gloves, can contain potentially endocrine disrupting chemicals, such as di-2-ethylhexyl phthalate (DEHP, CAS: 117-81-7). To investigate the contribution of FCM to dietary DEHP exposure we apply the product intake fraction (PiF: g intake/g in product) – a metric accounting for human intake of chemical mass per unit of mass embodied within a product. PiF of ingestion of DEHP is estimated from empirical data for PET water bottles on the order of 1E-7 through 1E-5 and for food handling gloves from 1E-6 for rice and 1E-3 for radishes. The uncertainty is related to unknown information (chemical content in FCM), circumstances of use (e.g., food item), and any analytical uncertainty. Using PiF, maximum allowable concentrations of DEHP within water bottles and gloves were calculated with respect to regulatory thresholds. A hypothetical average PiF for the FCM sector was calculated via production volume and oral exposure doses estimated from NHANES data. In both cases the indication was gloves may contribute more to DEHP exposure when used with certain food items than bottled water. DEHP content in gloves greater than 5% would cause exceedance of US EPA threshold when used with certain food items, e.g., radishes based on PiF calculated here. The PiF used in this context has applications for regulations related to FCM and exposure assessments on a per unit kilo basis.
Consistently Integrating Life-Cycle Impact Metrics into Chemical Alternatives Assessment

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Fantke, P. (Intern), Jolliet, O. (Ekstern), McKone, T. (Ekstern)
Pages: 132-132
Publication date: 2015

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Title of host publication: Abstract book : Buzzing with science
Publisher: SETAC
Main Research Area: Technical/natural sciences

Defining product intake fraction to quantify and compare exposure to consumer products
There is a growing consciousness that exposure studies need to better cover near-field exposure associated with products use. To consistently and quantitatively compare human exposure to chemicals in consumer products, we introduce the concept of product intake fraction, as the fraction of a chemical within a product that is eventually taken in by the human population. This metric enables consistent comparison of exposures during consumer product use for different product-chemical combinations, exposure duration, exposure routes and pathways and for other life cycle stages. We present example applications of the product intake fraction concept, for two chemicals in two personal care products and two chemicals encapsulated in two articles, showing how intakes of these chemicals can primarily occur during product use. We demonstrate the utility of the product intake fraction and its application modalities within life cycle assessment and risk assessment contexts. The product intake fraction helps to provide a clear interface between the life cycle inventory and impact assessment phases, to identify best suited sentinel products and to calculate overall exposure to chemicals in consumer products, or back-calculate maximum allowable concentrations of substances inside products.

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan
Authors: Jolliet, O. (Ekstern), Ernstoff, A. (Intern), Csiszar, S. A. (Ekstern), Fantke, P. (Intern)
Number of pages: 8
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Scopus rating (2014): SJR 2.777 SNIP 2.017
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.956 SNIP 2.103
ISI indexed (2013): ISI indexed yes
Developing, Applying, and Evaluating Models for Rapid Screening of Chemical Exposures

Chemical risk estimation requires quantitative information on exposures and toxicological effects. Quantitative exposure information can include chemical intake rates and (bio)monitoring data; however, such information does not exist for the vast majority of marketed chemicals. In addition to limited exposure data there is limited information on chemical use patterns and production and emission quantities. These data gaps require the application of mass balance, statistical and quantitative structure-activity relationship (QSAR) models to predict exposure and exposure potential for humans and ecological receptors. Models and modelling frameworks that can be parameterized and used for high-throughput screening (HTS) with the currently available (limited) chemical information are being developed and evaluated to obtain essential estimates of exposure for data poor chemicals. This presentation provides an introduction to underlying principles of some models used for exposure- and risk-based HTS for chemical prioritization for human health, including tools used in the ExpoDat project (USEtox, RAIDAR, CalTox) and other initiatives (SHEDS-HT). Case study examples of HTS include(i) model applications for screening thousands of chemicals for far-field human exposure, (ii) comparisons of far-field and near-field human exposure model results, and (iii) model evaluations with biomonitoring and monitoring data. These illustrations show how the current tools can be used in a regulatory setting and what improvements in the models and chemical information used to parameterize the models are needed to address uncertainty in HTS exposure estimation.

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, ARC Arnot Research & Consulting Inc., Harvard University, University of California, Davis, Hamner Institutes for Health Sciences
Authors: Arnot, J. (Ekstern), Shin, H. (Ekstern), Ernstoff, A. (Intern), Csiszar, S. A. (Ekstern), Fantke, P. (Intern), Zhang, X. (Ekstern), Bennett, D. (Ekstern), Jolliet, O. (Ekstern), Wetmore, B. (Ekstern), McKone, T. (Ekstern)
Number of pages: 1
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Dynamic toxicity modelling based on the USEtox matrix framework

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Fantke, P. (Intern), Jolliet, O. (Intern), Wannaz, C. (Ekstern)
Pages: 33-34
Publication date: 2015

Evaluating use stage exposure to food contact materials in a LCA framework
We present novel methods to incorporate exposure to chemicals within food contact materials (FCM) (e.g. packaging) into life cycle impact assessment (LCIA). Chemical migration into food is modeled as a function of contact temperature, time, and various chemical, FCM, and food properties. In order to reduce computing time and complexity, a double exponential curve was fit ($R^2$=1) to an exposure model which otherwise requires numeric solutions. The model is modified to evaluate the product intake fraction, $PiF$, which is a new metric that accounts for exposure to mass of chemicals embodied in a product in a way compatible with intake fraction, $iF$, a metric traditionally used in LCIA. The model predicts $PiF$ increases with temperature and for compounds with lower octanol-water partition coefficients within more permeable materials which are in contact with foods with high ethanol equivalencies (fatty foods).

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Ernstoff, A. (Intern), Jolliet, O. (Ekstern), Fantke, P. (Intern)
Pages: 311-314
Publication date: 2015

Exploring consumer exposure pathways and patterns of use for chemicals in the environment
Humans are exposed to thousands of chemicals in the workplace, home, and via air, water, food, and soil. A major challenge in estimating chemical exposures is to understand which chemicals are present in these media and microenvironments. Here we describe the Chemical/Product Categories Database (CPCat), a new, publically available
(http://actor.epa.gov/cpcat) database of information on chemicals mapped to “use categories” describing the usage or function of the chemical. CPCat was created by combining multiple and diverse sources of data on consumer- and industrial-process based chemical uses from regulatory agencies, manufacturers, and retailers in various countries. The database uses a controlled vocabulary of 833 terms and a novel nomenclature to capture and streamline descriptors of chemical use for 43,596 chemicals from the various sources. Examples of potential applications of CPCat are provided, including identifying chemicals to which children may be exposed and to support prioritization of chemicals for toxicity screening. CPCat is expected to be a valuable resource for regulators, risk assessors, and exposure scientists to identify potential sources of human exposures and exposure pathways, particularly for use in high-throughput chemical exposure assessment.

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, U.S. Environmental Protection Agency, North Carolina State University, Lockheed-Martin Research Laboratories
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**Exposure modeling of chemicals in personal care products**

**General information**

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Hamner Institutes for Health Sciences, University of Michigan
Authors: Csiszar, S. A. (Ekstern), Ernstoff, A. (Intern), Wetmore, B. (Ekstern), Fantke, P. (Intern), Jolliet, O. (Ekstern)
Pages: 50
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**From Incremental to Fundamental Chemical Substitution: Addressing the Lock-in Problem**

**General information**

State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Leuphana University of Lüneburg
Authors: Scheringer, M. (Ekstern), Fantke, P. (Intern), Weber, R. (Ekstern)
Pages: 117-117
From incremental to fundamental substitution in chemical alternatives assessment

Several chemicals in consumer products are subject to binding or voluntary phase-out agreements that are based on international treaties such as the Stockholm Convention on Persistent Organic Pollutants or on regulatory frameworks such as the European Union's Registration, Evaluation, Authorization and Restriction of Chemicals (REACH). To facilitate a phase-out process, alternatives assessment is commonly applied as an emerging approach to identifying chemicals (or materials, processes, and behavior changes) serving as substitutes. Polybrominated diphenyl ethers (PBDEs), long-chain poly- and perfluorinated alkyl substances (PFASs), and polychlorinated biphenyls (PCBs) are well-known cases of chemicals where substitution processes can be studied. Currently, there are various challenges in assessing, evaluating and effectively introducing chemical alternatives. These challenges are mainly related to similarity in chemical structures and, hence, similar hazard profiles between phase-out and substitute chemicals, leading to a rather incremental than fundamental substitution. A hampered phase-out process, the lack of implementing Green Chemistry principles in chemicals design, and lack of Sustainable Chemistry aspects in industrial processes design constitute additional challenges. We illustrate the various challenges in the process of phasing out and successfully substituting hazardous chemicals in consumer products and provide guiding principles for addressing these challenges. We propose an integrated approach of all stakeholders involved toward more fundamental and function-based substitution by greener and more sustainable alternatives. Our recommendations finally constitute a starting point for identifying further research needs and for improving current alternatives assessment practice.

Health effects of fine particulate matter in life cycle impact assessment: findings from the Basel Guidance Workshop

Purpose Fine particulate matter (PM$_{2.5}$) is considered to be one of the most important environmental factors contributing to the global human disease burden. However, due to the lack of broad consensus and harmonization in the life cycle assessment (LCA) community, there is no clear guidance on how to consistently include health effects from PM$_{2.5}$ exposure in LCA practice. As a consequence, different models are currently used to assess life cycle impacts for PM$_{2.5}$, sometimes leading to inconsistent results. In a global effort initiated by the United Nations Environment Programme (UNEP)/Society for Environmental Toxicology and Chemistry (SETAC) Life Cycle Initiative, respiratory inorganics’ impacts expressed as health effects from PM$_{2.5}$ exposure were selected as one of the initial impact categories to undergo review with the goal of providing global guidance for implementation in life cycle impact assessment (LCIA). The goal of this paper is to summarize the current knowledge and practice for assessing health effects from PM$_{2.5}$ exposure and to provide recommendations for their consistent integration into LCIA. Methods A task force on human health impacts was convened to build the framework for consistently quantifying health effects from PM$_{2.5}$ exposure and for recommending
PM$_{2.5}$ characterization factors. In an initial Guidance Workshop, existing literature was reviewed and input from a broad range of internationally recognized experts was obtained and discussed. Workshop objectives were to identify the main scientific questions and challenges for quantifying health effects from PM$_{2.5}$ exposure and to provide initial guidance to the impact quantification process. Results and discussion A set of 10 recommendations was developed addressing (a) the general framework for assessing PM$_{2.5}$-related health effects, (b) approaches and data to estimate human exposure to PM$_{2.5}$ using intake fractions, and (c) approaches and data to characterize exposure-response functions (ERFs) for PM$_{2.5}$ and to quantify severity of the diseases attributed to PM$_{2.5}$ exposure. Despite these advances, a number of complex issues, such as those related to non-linearity of the ERFs and the possible need to provide different ERFs for use in different geographical regions, require further analysis. Conclusions and outlook Questions of how to refine and improve the overall framework were analyzed. Data and models were proposed for harmonizing various elements of the health impact pathways for PM$_{2.5}$. Within the next two years, our goal is to build a global guidance framework and to determine characterization factors that are more reliable for incorporating the health effects from exposure to PM$_{2.5}$ into LCA. Ideally, this will allow quantification of the impacts of both indoor and outdoor exposures to PM$_{2.5}$.
Human Toxicity

This chapter reviews the human toxicological impacts of chemicals and how to assess these impacts in life cycle impact assessment (LCIA), in order to identify key processes and pollutants. The complete cause-effect pathway – from emissions of toxic substances up to damages on human health – demonstrates the importance to account for both outdoor and indoor exposure, including consumer products. Analysing the variations in intake fraction (the fraction of the emitted or applied chemical that is taken in by the consumer and the general population), effect factor and characterisation factor across all chemicals and impact pathways characterizes the contribution of each factor to the total variation of 10–12 orders of magnitude in impacts per kg across all chemicals. This large variation between characterisation factors for different chemicals as well as the 3 orders of magnitude uncertainty on characterisation factors means that results should by default be reported and interpreted in log scales when comparing scenarios or substance contribution! We conclude by outlining future trends in human toxicity modelling for LCIA, with promising developments for (a) better estimates of degradation half-lives, (b) the inclusion of ionization of chemicals in human exposure including bioaccumulation, (c) metal speciation, (d) spatialised models to differentiate the variability associated with spatialisation from the uncertainty, and (e) the assessment of chemical exposure via consumer products and occupational settings. As a whole, the assessment of toxicity in LCA has progressed on a very sharp learning curve during the past 20 years. This rapid progression is expected to continue in the coming years, focusing more on direct exposure of workers to chemicals during manufacturing and of consumers during product use. The first section of this chapter outlines the complete cause-effect pathway, from emissions of toxic substances to intake by the population up to damages in terms of human health effects. Section 2 outlines the framework for assessing human toxicity in LCIA. Section 3 discusses the contributing substances and their coverage in LCIA methods. Section 4 provides an overview of the main LCIA methods available to address human toxicological impacts. Section 5 presents the range of variation of factor across chemicals, the main sources of uncertainty and good interpretation practice of results from human toxicity assessments. Section 6 finally discusses new developments and research needs.

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Authors: Jolliet, O. (Ekstern), Fantke, P. (Intern)
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Particulate Matter Formation

This chapter deals with the causes and consequences of exposure from emissions of primary particles and secondary particle precursors on human health and how to deal with them in life cycle impact assessment (LCIA). Following a short introduction and literature review, the first part outlines the complete emission-to-damage pathway, from emissions of primary particles and secondary particle precursors to damage on human health, so called 'respiratory effects from particles'. It describes the assessment framework for quantifying respiratory effects from particles in the context of LCIA. The second part provides an overview of methods that have been available in LCA to address impact of particles on human health. We finally discuss variability and main sources of uncertainties, as well as future trends in modelling respiratory effects of particles in LCIA.

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Humbert, S. (Ekstern), Fantke, P. (Intern), Jolliet, O. (Ekstern)
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Pesticide Substitution: Combining Food Safety with Environmental Quality

Various pesticides are authorized for use on agricultural food crops. Despite regulatory risk assessments aiming at ensuring consumer and environmental safety, pesticides contribute to human and environmental impacts. Guidance is needed to optimize pesticide use practice and minimize human and environmental exposure. Comparative pesticide substitution scenarios are presented to address this need. In a case study on wheat, different pesticides have been compared with respect to their substitution potential with focus on human health. Results demonstrate that health impacts can be reduced up to 99% by defining adequate substitution scenarios. Comprehensive scenarios need to also consider worker and environmental burden, and information on crop rotation, pest pressure, environmental conditions, application costs and efficacy. Such scenarios help to increase food safety and more sustainable use of pesticides.

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Fantke, P. (Intern)
Pages: 291-293
Risk-based high-throughput chemical screening and prioritization using exposure models and in vitro bioactivity assays

We present a risk-based high-throughput screening (HTS) method to identify chemicals for potential health concerns or for which additional information is needed. The method is applied to 180 organic chemicals as a case study. We first obtain information on how the chemical is used and identify relevant use scenarios (e.g., dermal application, indoor emissions). For each chemical and use scenario, exposure models are then used to calculate a chemical intake fraction, or a product intake fraction, accounting for chemical properties and the exposed population. We then combine these intake fractions with use scenario-specific estimates of chemical quantity to calculate daily intake rates (IR; mg/kg/day). These intake rates are compared to oral equivalent doses (OED; mg/kg/day), calculated from a suite of ToxCast in vitro bioactivity assays using in vitro-to-in vivo extrapolation and reverse dosimetry. Bioactivity quotients (BQs) are calculated as IR/OED to obtain estimates of potential impact associated with each relevant use scenario. Of the 180 chemicals considered, 38 had maximum IRs exceeding minimum OEDs (i.e., BQs > 1). For most of these compounds, exposures are associated with direct intake, food/oral contact, or dermal exposure. The method provides high-throughput estimates of exposure and important input for decision makers to identify chemicals of concern for further evaluation with additional information or more refined models.

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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.777 SNIP 2.017
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ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.146 SNIP 2.056
ISI indexed (2012): ISI indexed yes
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The Glasgow consensus on the delineation between pesticide emission inventory and impact assessment for LCA

Pesticides are applied to agricultural fields to optimise crop yield and their global use is substantial. Their consideration in life cycle assessment (LCA) is affected by important inconsistencies between the emission inventory and impact assessment phases of LCA. A clear definition of the delineation between the product system model (life cycle inventory—LCI, technosphere) and the natural environment (life cycle impact assessment—LCIA, ecosphere) is missing and could be established via consensus building. A workshop held in 2013 in Glasgow, UK, had the goal of establishing consensus and creating clear guidelines in the following topics: (1) boundary between emission inventory and impact characterisation model, (2) spatial dimensions and the time periods assumed for the application of substances to open agricultural fields or in greenhouses and (3) emissions to the natural environment and their potential impacts. More than 30 specialists in agrifood LCI, LCIA, risk assessment and ecotoxicology, representing industry, government and academia from 15 countries and four continents, met to discuss and reach consensus. The resulting guidelines target LCA practitioners, data (base) and characterisation method developers, and decision makers. The focus was on defining a clear interface between LCI and LCIA, capable of supporting any goal and scope requirements while avoiding double counting or exclusion of important emission flows/impacts. Consensus was reached accordingly on distinct sets of recommendations for LCI and LCIA, respectively, recommending, for example, that buffer zones should be considered as part of the crop production system and the change in yield be considered. While the spatial dimensions of the field were not fixed, the temporal boundary between dynamic LCI fate modelling and steady-state LCIA fate modelling needs to be defined. For pesticide application, the inventory should report pesticide identification, crop, mass applied per active ingredient, application method or formulation type, presence of buffer zones, location/country, application time before harvest and crop growth stage during application, adherence with Good Agricultural Practice, and whether the field is considered part of the technosphere or the ecosphere. Additionally, emission fractions to environmental media on-field and off-field should be reported. For LCIA, the directly concerned impact categories and a list of relevant fate and exposure processes were identified. Next steps were identified: (1) establishing default emission fractions to environmental media for integration into LCI databases and (2) interaction among impact model developers to extend current methods with new elements/processes mentioned in the recommendations.

General information

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Food Security, Quantis, Syngenta Crop Protection, Interuniversity Research Centre for the Life Cycle of Products, Processes and Services, Tropical Pesticides Research Institute

Authors: Rosenbaum, R. K. (Intern), Anton, A. (Ekstern), Bengoa, X. (Ekstern), Bjørn, A. (Intern), Brain, R. (Ekstern), Bulle, C. (Ekstern), Cosme, N. M. D. (Intern), Dijkman, T. J. (Intern), Fantke, P. (Intern), Felix, M. (Ekstern)
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The Role of Dissipation Processes in Plants for Modeling Bioaccumulation

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Authors: Fantke, P. (Intern), Trapp, S. (Intern), Amot, J. (Ekstern), Doucette, W. (Ekstern)
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The USEtox story: A survey of model developer visions and user requirements
Purpose USEtox is a scientific consensus model for assessing human toxicological and ecotoxicological impacts that is widely used in life cycle assessment (LCA) and other comparative assessments. However, how user requirements are met has never been investigated. To guide future model developments, we analyzed user expectations and experiences and compared them with the developers’ visions.
Methods We applied qualitative and quantitative data collection methods including an online questionnaire, semi-structured user and developer interviews, and review of scientific literature. Questionnaire and interview results were analyzed in an actor-network perspective in order to understand user needs and to compare these with the developers’ visions. Requirement engineering methods, more specifically function tree, system context, and activity diagrams, were iteratively applied and structured to develop specific user requirements-driven recommendations for setting priorities in future USEtox development and for discussing general implications for developing scientific models.
Results and discussion The vision behind USEtox was to harmonize available data and models for assessing toxicological impacts in LCA and to provide global guidance for practitioners. Model developers show different perceptions of some underlying aspects including model transparency and expected user expertise. Users from various sectors and geographic regions apply USEtox mostly in research and for consulting. Questionnaire and interview results uncover various user requests regarding USEtox usability. Results were systematically analyzed to translate user requests into recommendations to improve USEtox from a user perspective and were afterwards applied in the further USEtox development process.
Conclusions We demonstrate that understanding interactions between USEtox and its users helps guiding model development and dissemination. USEtox-specific recommendations are to (1) respect the application context for different user types, (2) provide detailed guidance for interpreting model and factors, (3) facilitate consistent integration into LCA software and methods, (4) improve update/testing procedures, (5) strengthen communication between developers and users, and (6) extend model scope. By generalizing our recommendations to guide scientific model development in a broader context, we emphasize to acknowledge different levels of user expertise to integrate sound revision and update procedures and to facilitate modularity, data import/export, and incorporation into relevant software and databases during model design and development. Our fully documented approach can inspire performing similar surveys on other LCA-related tools to consistently analyze user requirements and provide improvement recommendations based on scientific user analysis methods.

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Westh, T. B. (Intern), Hauschild, M. Z. (Intern), Birkved, M. (Intern), Jørgensen, M. S. (Intern), Rosenbaum, R. K. (Intern), Fantke, P. (Intern)
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Commonwealth Scientific and Industrial Research Organisation, ETH Zurich, University of Texas, Norwegian University of Science and Technology, United Nations Environmental Programme, University of Western Sydney, Oxford Brookes University, European Commission - Joint Research Center, University of New South Wales
Authors: Ridoutt, B. (Ekstern), Fantke, P. (Intern), Pfister, S. (Ekstern), Bare, J. (Ekstern), Boulay, A. (Ekstern), Cherubini, F. (Ekstern), Frischknecht, R. (Ekstern), Hauschild, M. Z. (Intern), Hellweg, S. (Ekstern), Henderson, A. (Ekstern), Jolliet, O. (Ekstern), Levasseur, A. (Ekstern), Margni, M. (Ekstern), McKone, T. E. (Ekstern), Michelsen, O. (Ekstern), i Canals, L. M. (Ekstern), Page, G. (Ekstern), Pant, R. (Ekstern), Raugei, M. (Ekstern), Sala, S. (Ekstern), Saouter, E. (Ekstern), Verones, F. (Ekstern), Wiedmann, T. (Ekstern)
Confronting Health Effects of Particulate Matter in LCIA

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan, University of California
Authors: McKone, T. (Ekstern), Fantke, P. (Intern), Jolliet, O. (Ekstern)
Considering human exposure to pesticides in food products: Importance of dissipation dynamics

The general public is continuously concerned about effects from pesticide exposure via residues in food crops. However, impacts from pesticide exposure are mostly neglected in food product-related LCAs. Time-to-harvest and dissipation from crops mainly drive residue dynamics with dissipation as most uncertain aspect in characterization modeling. We analyzed measured half-lives (n=4513) with 95% falling between 0.6 and 29 days. With ~500 pesticides authorized alone in the EU for several hundred crops, however, experimental studies only cover few possible pesticide-crop combinations. Therefore, we estimated dissipation from measured data and provide reference half-lives for 333 pesticides applied at 20°C under field conditions. Our framework allows for detailed explorations of dietary choices in LCA with respect to human health impacts from pesticide exposure via crop consumption. The next step is to include pesticide exposure via crop consumption along with improved pesticide dissipation data into existing LCIA methodologies for consideration in future LCA studies.

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Dr. Knoell Consult GmbH
Authors: Fantke, P. (Intern), Juraske, R. (Ekstern), Jolliet, O. (Ekstern)
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Source: PublicationPreSubmission
Developing and applying high-throughput exposure models for screening-level chemical assessment: The ExpoDat project

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Arnot, J. (Exkstern), Ernstoff, A. (Intern), Shin, H. (Exkstern), Csizar, S. (Exkstern), Fantke, P. (Intern), Zhang, X. (Exkstern), Jolliet, O. (Exkstern), Bennett, D. (Exkstern), Wetmore, B. (Exkstern)
Publication date: 2014
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Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Direct Exposure of Consumers to Personal Care Products

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan
Authors: Jolliet, O. (Exkstern), Ernstoff, A. (Intern), Csiszar, S. A. (Exkstern), Fantke, P. (Intern)
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Publisher: International Society of Exposure Science
Main Research Area: Technical/natural sciences
Electronic versions:
Direct_Exposure_of_Consumers.pdf
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Estimating Half-Lives for Pesticide Dissipation from Plants

Pesticide risk and impact assessment models critically rely on and are sensitive to information describing dissipation from plants. Despite recent progress, experimental data are not available for all relevant pesticide–plant combinations, and currently no model predicting plant dissipation accounts for the influence of substance properties, plant characteristics, temperature, and study conditions. In this study, we propose models to estimate half-lives for pesticide dissipation from plants and provide recommendations for how to use our results. On the basis of fitting experimental dissipation data with reported average air temperatures, we estimated a reaction activation energy of 14.25 kJ/mol and a temperature coefficient Q10 of 1.22 to correct dissipation from plants for the influence of temperature. We calculated a set of dissipation half-lives for 333 substances applied at 20 °C under field conditions. Half-lives range from 0.2 days for pyrethrins to 31 days for dalapon. Parameter estimates are provided to correct for specific plant species, temperatures, and study conditions. Finally, we propose a predictive regression model for pesticides without available measured dissipation data to estimate half-lives based on substance properties at the level of chemical substance class. Estimated half-lives from our study are designed to be applied in risk and impact assessment models to either directly describe dissipation or as first proxy for describing degradation.

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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan, Dr. Knoell Consult GmbH
Authors: Fantke, P. (Intern), Gillespie, B. W. (Ekstern), Juraske, R. (Ekstern), Jolliet, O. (Ekstern)
Pages: 8588–8602
Publication date: 2014
Exposure and Toxicity Modeling of Chemicals in Personal Care Products: Case Study Using Parabens

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan
Authors: Csiszar, S. A. (Ekstern), Ernstoff, A. (Intern), Fantke, P. (Intern), Richardson, R. (Ekstern), Jolliet, O. (Ekstern)
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Flagging health risks of chemicals by combining in vitro bioactivity data with environmental and consumer product exposure modeling

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of California, Davis, University of Toronto
Authors: Ernstoff, A. (Intern), Shin, H. (Ekstern), Bennett, D. (Ekstern), Arnot, J. (Ekstern), Csiszar, S. (Ekstern), Fantke, P. (Intern), Wetmore, B. (Ekstern), Jolliet, O. (Ekstern)
Number of pages: 1
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Global guidance on environmental life cycle impact assessment indicators: findings of the scoping phase

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan, treeze Ltd., Ecole Polytechnique de Montreal, King Mongkut’s University of Technology Thonburi, Tokyo City University, University of California, Unilever, National Institute of Public Health and the Environment, Arizona State University, Commonwealth Scientific and Industrial Research Organisation, University of Bordeaux, Radboud Universiteit, SETAC, Procter and Gamble, U.S. Environmental Protection Agency
Authors: Jolliet, O. (Ekstern), Frischknecht, R. (Ekstern), Bare, J. (Ekstern), Boulay, A. (Ekstern), Bulle, C. (Ekstern), Fantke, P. (Intern), Gheewala, S. (Ekstern), Hauschild, M. Z. (Intern), Itsubo, N. (Ekstern), Margni, M. (Ekstern), McKone, T. E. (Ekstern), Canals, L. M. Y. (Ekstern), Posthuma, L. (Ekstern), Prado-Lopez, V. (Ekstern), Ridoutt, B. (Ekstern), Sonnemann, G. (Ekstern), Rosenbaum, R. K. (Intern), Seager, T. (Ekstern), Struijs, J. (Ekstern), Zelm, R. V. (Ekstern), Vigon, B. (Ekstern), Weisbrod, A. (Ekstern)
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BFI (2016): BFI-level 2
Scopus rating (2016): SJR 1.328 SNIP 1.423
BFI (2015): BFI-level 2
How can we avoid the lock-in problem in the substitution of hazardous chemicals used in consumer products?

A wide range of chemical substances is used in consumer products for various purposes, including plastic softeners, dyestuffs and colorants, flame retardants, impregnation agents, antioxidants and UV absorbers, preservation agents and
biocides, and many others. Among these chemicals, there is a certain fraction of substances with hazardous properties such as persistence, bioaccumulation potential and toxicity (PBT properties) or the ability to interfere with the hormonal system (endocrine disrupting chemicals, EDCs). Large-scale screening exercises have shown that there may be several hundreds of chemicals with PBT properties among the several tens of thousands of substances on the market. There are some groups of chemicals that have raised particular concerns such as polybrominated diphenyl ethers (PBDEs) or long-chain poly and perfluorinated alkyl substances (PFASs). These substances have been regulated or are subject to voluntary phase-out programs; specifically, penta- and octabrominated BDEs are scheduled for elimination globally under the Stockholm Convention on Persistent Organic Pollutants; uses of perfluorooctane sulfonic acid (PFOS) are being restricted under the Stockholm Convention, and perfluorooctanoic acid (PFOA) and C_{11}–C_{14} fluorocarboxylic acids are regulated in the European Union as PBT substances and vPvB (very persistent, very bioaccumulative) substances, respectively. In addition, all long-chain PFASs (substances with seven or more perfluorinated carbons) are subject of voluntary phase-out programs conducted by major producers of fluoropolymers and fluorotelomer-based products. However, it has become evident that the replacements of these substances include chemically similar substances, i.e. brominated aromatic substances in the case of PBDEs and shorter-chain PFASs in the case of long-chain PFASs. These are two examples of a substitution process that leads to an incremental rather than a fundamental change in the structure of chemicals used in consumer products. Here we discuss the conditions for incremental and fundamental changes in the substitution process of chemicals.

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State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, POPs Environmental Consulting
Authors: Scheringer, M. (Ekstern), Fantke, P. (Intern), Weber, R. (Ekstern)
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How can we avoid the lock-in problem in the substitution of hazardous chemicals used in consumer products?
A wide range of chemical substances is used in consumer products for various purposes, including plastic softeners, dyestuffs and colorants, flame retardants, impregnation agents, antioxidants and UV absorbers, preservation agents and biocides, and many others. Among these chemicals, there is a certain fraction of substances with hazardous properties such as persistence, bioaccumulation potential and toxicity (PBT properties) or the ability to interfere with the hormonal system (endocrine disrupting chemicals, EDCs). Large-scale screening exercises have shown that there may be several hundreds of chemicals with PBT properties among the several tens of thousands of substances on the market. There are some groups of chemicals that have raised particular concerns such as polybrominated diphenyl ethers (PBDEs) or long-chain poly and perfluorinated alkyl substances (PFASs). These substances have been regulated or are subject to voluntary phase-out programs; specifically, penta- and octabrominated BDEs are scheduled for elimination globally under the Stockholm Convention on Persistent Organic Pollutants; uses of perfluorooctane sulfonic acid (PFOS) are being restricted under the Stockholm Convention, and perfluorooctanoic acid (PFOA) and C_{11}–C_{14} fluorocarboxylic acids are regulated in the European Union as PBT substances and vPvB (very persistent, very bioaccumulative) substances, respectively. In addition, all long-chain PFASs (substances with seven or more perfluorinated carbons) are subject of voluntary phase-out programs conducted by major producers of fluoropolymers and fluorotelomer-based products. However, it has become evident that the replacements of these substances include chemically similar substances, i.e. brominated aromatic substances in the case of PBDEs and shorter-chain PFASs in the case of long-chain PFASs. These are two examples of a substitution process that leads to an incremental rather than a fundamental change in the structure of chemicals used in consumer products. Here we discuss the conditions for incremental and fundamental changes in the substitution process of chemicals.

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, POPs Environmental Consulting
Authors: Scheringer, M. (Ekstern), Fantke, P. (Intern), Weber, R. (Ekstern)
Incorporating Health Impacts from Exposure to Chemicals in Food Packaging in LCA

Life cycle assessments (LCA) on the environmental and public health impacts of food and beverage packaging materials have found some advantages to plastic over glass. Entirely missing from these evaluations are the health impacts of possible chemical, e.g., endocrine dis-ruptor, exposure through migration of chemicals from the packaging into the food product. We build a framework based on a life cycle perspective to predict which chemicals may be in a package that are not intentionally added ingredients, and we apply this approach to the US EPA’s CPCAT database. In total we find 1,154 chemicals within the CPCAT database related to food-contact materials; out of these 107 are potential endocrine disruptors according to the TEDX list of endocrine disruptors. We also build a framework in an effort to begin harmonizing LCA to include health impacts of chemical exposure related to food packaging in conjunction with other traditional LCA environmental impact categories.
Integrating nutritional benefits and impacts in a life cycle assessment framework: A US dairy consumption case study

Although essential to understand the overall health impact of a food or diet, nutrition is not usually considered in food-related life cycle assessments (LCAs). As a case study to demonstrate comparing environmental and nutritional health impacts we investigate United States dairy consumption. Nutritional impacts, interpreted from disease burden epidemiology, are compared to health impacts from more traditional impacts (e.g. due to exposure to particulate matter emissions across the life cycle) considered in LCAs. After accounting for the present consumption, data relating dairy intake to public health suggest that low-fat milk leads to nutritional benefits up to one additional daily serving in the American diet. We demonstrate the importance of considering the whole-diet and nutritional trade-offs. The estimated health impacts of various dietary scenarios may be of comparable magnitude to environmental impacts suggesting the need for investigating the balance between dietary public health advantages and disadvantages in comparison to environmental impacts.

Screening human health risk of environmental and direct exposure to personal care products

Substitution and food: Toward more sustainable pesticide use
SWITCH-Med SCP Policy Toolkit: Mainstreaming Sustainable Consumption and Production into Key Economic Sectors in the Mediterranean

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Centre for Sustainable Development Solutions, Egypt National Cleaner Production Centre, Institute for Global Environmental Strategies, Lebanese Centre for Energy Conservation, United Nations Environmental Programme, Andalusian Institute of Technology, Global Footprint Network, Ministry of Environmental and Nature Protection, Collaborating Centre on Sustainable Consumption and Production, Ministry of Agriculture, Natural Resources and Environment, Ministry of Sustainable Development and Tourism, Ministry of Environmental Protection, Environment and Planning Authority, GFA Consulting Group, Hydro-Engineering Institute, Cleaner Technology Centre, Priority Actions Programme/Regional Activity Centre, Agenzia regionale Conservatoria delle Coste della Sardegna, POPs Environmental Consulting, Centre National des Technologies de Production plus Propre
Authors: Abaza, H. (Ekstern), Sena, A. A. (Ekstern), Akenji, L. (Ekstern), El Khoury, P. (Ekstern), Fantke, P. (Intern), Fotiou, S. (Ekstern), Furphy, A. D. (Ekstern), Galli, A. (Ekstern), Guberina, B. G. (Ekstern), Guillén, G. (Ekstern), Hajipakkos, C. (Ekstern), Knezevic, J. (Ekstern), Koundis, S. (Ekstern), Laster, Y. (Ekstern), Lauwers, F. (Ekstern), Mansour, L. (Ekstern), Midzic-Kurtagic, S. (Ekstern), Novak, B. P. (Ekstern), Pizzuto, A. (Ekstern), Prem, M. (Ekstern), Reuter, L. (Ekstern), Satta, A. (Ekstern), Tuncer, B. (Ekstern), Vázquez, V. (Ekstern), Vespeek, F. (Ekstern), Weber, R. (Ekstern), Zouaoui, A. (Ekstern)
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Variability and uncertainty of intake fraction as a function of distance from source

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Wannaz, C. (Ekstern), Jolliet, O. (Ekstern), Fantke, P. (Intern)
Pages: 225-226
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Characterizing pesticide dissipation in food crops

Ingestion of residues via consumption of food crops is the predominant exposure route of the general population toward pesticides. However, pesticide dissipation in crops constitutes a main source of uncertainty in estimating residues in harvested crop parts and subsequent human exposure. Nevertheless, dissipation is a key mechanism in models assessing pesticide distribution in the crop environment and the magnitude of residues in harvest. We provide a consistent framework for characterizing pesticide dissipation in food crops for use in modeling approaches applied in health risk and impact assessment. We collected 4,482 unique dissipation half-lives for 341 substances applied to 182 different crop species and fully characterize these data by describing their variance, distribution and uncertainty as well as by identifying the influence of substance, crop and environmental characteristics. We obtain an overall geo-mean half-life over all data points of 3.9 days with 95% of all half-lives falling within the range between 0.6 and 29 days. Uncertainty in predicting a substance-specific geo-mean half-life varies with varying numbers of available data points with the highest uncertainty associated to pesticides with less than seven reported half-lives. Temperature in air was identified to have a significant influence on dissipation kinetics. We, hence, provide estimated half-lives for a default temperature of 20°C, while introducing a correction term for deviating temperature conditions. Diffusive exchange processes also have a significant...
influence on pesticide dissipation, wherever these processes dominate dissipation rates compared to degradation. In these cases, we recommend not to use measured dissipation half-lives as basis for estimating degradation, which is recommended in cases, where degradation is dominating. We are currently testing the regression to predict degradation half-lives in crops. By providing mean degradation half-lives at 20°C for more than 300 pesticides, we reduce uncertainty and improve assumptions in current practice of health risk and impact assessments.

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State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Swiss Federal Institute of Technology, University of Michigan
Authors: Fantke, P. (Intern), Juraske, R. (Ekstern), Jolliet, O. (Ekstern)
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Dynamics of pesticide uptake into plants: From system functioning to parsimonious modeling
Dynamic plant uptake models are suitable for assessing environmental fate and behavior of toxic chemicals in food crops. However, existing tools mostly lack in-depth analysis of system dynamics. Furthermore, no existing model is available as parameterized version that is easily applicable for use in spatially resolved frameworks for comparative assessment. In the present paper, we thus analyze the dynamics of substance masses in a multi-compartment plant–environment system by applying mathematical decomposition techniques. We thereby focus on the evolution of pesticide residues in crop components harvested for human consumption by taking wheat grains as example. Results show that grains, grain surface and soil are the compartments predominantly influencing the mass evolution of most pesticides in the plant–environment system as a function of substance degradation in plant components and overall residence time in soil. Additional influences are associated with substance molecular weight and time span between pesticide application and crop harvest. Building on these findings, we provide an accurate and yet simple linear approximation of the dynamical system to predict masses in harvested crop components relative to the total applied pesticide, defined as harvest fractions. Parameterized predictions correspond well with results from the full dynamic model, with an overall deviation of a factor 22 for harvest fractions in the relevant range between 1 and 10−10 in wheat. The in-depth analysis of model dynamics provides additional information of the evolution of pesticides in food crops, which is important for regulators and practitioners. In addition, the parametric representation of system dynamics allows for drastically reducing input data requirements and for comparing harvest fractions of a wide range of substances without using a complex dynamic model.

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Stuttgart, University of Michigan, University of Stuttgart, École Polytechnique Fédérale de Lausanne
Authors: Fantke, P. (Intern), Wieland, P. (Ekstern), Wannaz, C. (Ekstern), Friedrich, R. (Ekstern), Jolliet, O. (Ekstern)
Pages: 316-324
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Main Research Area: Technical/natural sciences

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BFI (2016): BFI-level 2
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.119 SNIP 2.172
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.065 SNIP 2.483
Keeping USEtox up-to-date: What is coming and how you can contribute

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Prioritizing consumer product categories based on exposure estimates

General information
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Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, University of Michigan
Authors: Ernstoff, A. (Intern), Fantke, P. (Intern), Jolliet, O. (Ekstern)
Pages: 56-57
Publication date: 2013

Host publication information
Variability of Pesticide Dissipation Half-Lives in Plants

Information on dissipation kinetics of pesticides in food crops and other plants is a key aspect in current risk and impact assessment practice. This is because human exposure to pesticides is predominantly caused by residues in agricultural crops grown for human and animal consumption. However, modeling dissipation of pesticides in plants is highly uncertain and therefore strongly relies on experimental data. Unfortunately, available information on pesticide dissipation in plants from experimental studies only covers a small fraction of possible combinations of substances authorized for use on food and fodder crops. Additionally, aspects and processes influencing dissipation kinetics are still not fully understood. Therefore, we systematically reviewed 811 scientific literature sources providing 4513 dissipation half-lives of 346 pesticides measured in 183 plant species. We focused on the variability across substances, plant species and harvested plant components and finally discuss different substance, plant and environmental aspects influencing pesticide dissipation. Measured half-lives in harvested plant materials range from around 1 hour for pyrethrins in leaves of tomato and pepper fruit to 918 days for pyriproxyfen in pepper fruits under cold storage conditions. Ninety-five percent of all half-lives fall within the range between 0.6 and 29 days. Our results emphasize that future experiments are required to analyze pesticide–plant species combinations that have so far not been covered and that are relevant for human exposure. In addition, prediction models would help to assess all possible pesticide–plant species combinations in the context of comparative studies. The combination of both would finally reduce uncertainty and improve assumptions in current risk and impact assessment practice.

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Authors: Fantke, P. (Intern), Juraske, R. (Ekstern)
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Scopus rating (2015): SJR 2.584 SNIP 1.828
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.777 SNIP 2.017
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.956 SNIP 2.103
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 3.146 SNIP 2.056
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.178 SNIP 1.953
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.964 SNIP 1.729
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.835 SNIP 1.803
Deposition and residues of azoxystrobin and imidacloprid on greenhouse lettuce with implications for human consumption

Lettuce greenhouse experiments were carried out from March to June 2011 in order to analyze how pesticides behave from the time of application until their intake via human consumption taking into account the primary distribution of pesticides, field dissipation, and post-harvest processing. In addition, experimental conditions were used to evaluate a new dynamic plant uptake model comparing its results with the experimentally derived residues. One application of imidacloprid and two of azoxystrobin were conducted. For evaluating primary pesticide distribution, two approaches based on leaf area index and vegetation cover were used and results were compared with those obtained from a tracer test. High influence of lettuce density, growth stage and type of sprayer was observed in primary distribution showing that low densities or early growth stages implied high losses of pesticides on soil. Washed and unwashed samples of lettuce were taken and analyzed from application to harvest to evaluate removal of pesticides by food processing. Results show that residues found on the Spanish preharvest interval days were in all cases below officially set maximum residue limits, although it was observed that time between application and harvest is as important for residues as application amounts. An overall reduction of 40–60% of pesticides residues was obtained from washing lettuce. Experimentally derived residues were compared with modeled residues and deviate from 1.2 to 1.4 for imidacloprid and azoxystrobin, respectively, presenting good model predictions. Resulting human intake fractions range from 0.045kg intake kg applied⁻¹ for imidacloprid to 0.14kg intake kg applied⁻¹ for azoxystrobin.

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Authors: Itoiz, E. S. (Ekstern), Fantke, P. (Intern), Juraske, R. (Ekstern), Kounina, A. (Ekstern), Vallejo, A. A. (Ekstern)
Pages: 1034-1041
Publication date: 2012
Main Research Area: Technical/natural sciences

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Ratings:
BFI (2017): BFI-level 2
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 1.417 SNIP 1.606
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.51 SNIP 1.57
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.593 SNIP 1.651
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.724 SNIP 1.767
ISI indexed (2013): ISI indexed yes
Health impact and damage cost assessment of pesticides in Europe

Health impacts from pesticide use are of continuous concern in the European population, requiring a constant evaluation of European pesticide policy. However, health impacts have never been quantified accounting for specific crops contributing differently to overall human exposure as well as accounting for individual substances showing distinct environmental behavior and toxicity. We quantify health impacts and related damage costs from exposure to 133 pesticides applied in 24 European countries in 2003 adding up to almost 50% of the total pesticide mass applied in that year. Only 13 substances applied to 3 crop classes (grapes/vines, fruit trees, vegetables) contribute to 90% of the overall health impacts of about 2000 disability-adjusted life years in Europe per year corresponding to annual damage costs of 78 million Euro. Considering uncertainties along the full impact pathway mainly attributable to non-cancer dose–response relationships and residues in treated crops, we obtain an average burden of lifetime lost per person of 2.6 hours (95% confidence interval between 22 seconds and 45.3 days) or costs per person over lifetime of 12 Euro (95% confidence interval between 0.03 Euro and 5142 Euro), respectively. 33 of the 133 assessed substances accounting for 20% of health impacts in 2003 are now banned from the European market according to current legislation. The main limitation in assessing human health impacts from pesticides is related to the lack of systematic application data for all used substances. Since health impacts can be substantially influenced by the choice of pesticides, the need for more information about substance application becomes evident. © 2012 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Technical University of Denmark, University of Stuttgart, University of Michigan
Authors: Fantke, P. (Intern), Friedrich, R. (Ekstern), Jolliet, O. (Ekstern)
Pages: 9-17
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Environment International
Volume: 49
ISSN (Print): 0160-4120
Ratings:
BFI (2017): BFI-level 2
Parameterization Models for Pesticide Exposure via Crop Consumption

An approach for estimating human exposure to pesticides via consumption of six important food crops is presented that can be used to extend multimedia models applied in health risk and life cycle impact assessment. We first assessed the variation of model output (pesticide residues per kg applied) as a function of model input variables (substance, crop, and environmental properties) including their possible correlations using matrix algebra. We identified five key parameters responsible for between 80% and 93% of the variation in pesticide residues, namely time between substance application and crop harvest, degradation half-lives in crops and on crop surfaces, overall residence times in soil, and substance molecular weight. Partition coefficients also play an important role for fruit trees and tomato (Kow), potato (Koc), and lettuce (Kaw, Kow). Focusing on these parameters, we develop crop-specific models by parametrizing a complex fate and exposure assessment framework. The parametric models thereby reflect the framework’s physical and chemical mechanisms and predict pesticide residues in harvest using linear combinations of crop, crop surface, and soil compartments. Parametric model results correspond well with results from the complex framework for 1540 substance-crop combinations with total deviations between a factor 4 (potato) and a factor 66 (lettuce). Predicted residues also correspond well with experimental data previously used to evaluate the complex framework. Pesticide mass in harvest can finally be combined with reduction factors accounting for food processing to estimate human exposure from crop consumption. All parametric models can be easily implemented into existing assessment frameworks.
Pesticide residue dynamics in passion fruits: Comparing field trial and modelling results

We evaluated the exposure to pesticides from the consumption of passion fruits and subsequent human health risks by combining several methods: (i) experimental field studies including the determination of pesticide residues in/on passion fruits, (ii) dynamic plant uptake modelling, and (iii) human health risk assessment concepts. Eight commonly used pesticides were applied onto passion fruits cultivated in Colombia. Pesticide concentrations were measured periodically (between application and harvest) in whole fruits and fruit pulp. Measured concentrations were compared with predicted...
residues calculated with a dynamic and crop-specific pesticide uptake model, namely dynamiCROP. The model accounts for the time between pesticide application and harvest, the time between harvest and consumption, the amount of spray deposition on plant surfaces, uptake processes, dilution due to crop growth, degradation in plant components, and reduction due to food processing (peeling). Measured and modelled residues correspond well ($r^2=0.88–0.99$), with all predictions falling within the 90% confidence interval of the measured values. A mean error of 43% over all studied pesticides was observed between model estimates and measurements. The fraction of pesticide applied during cultivation that is eventually ingested by humans is on average $10^{-4}$–$10^{-6}$, depending on the time period between application and ingestion and the processing step considered. Model calculations and intake fractions via fruit consumption based on experimental data corresponded well for all pesticides with a deviation of less than a factor of 2. Pesticide residues in fruits measured at recommended harvest dates were all below European Maximum Residue Limits (MRLs) and therefore do not indicate any violation of international regulatory thresholds.

**General information**

State: Published
Organisations: Swiss Federal Institute of Technology, International Center for Tropical Agriculture, University of Stuttgart
Authors: Juraske, R. (Ekstern), Fantke, P. (Intern), Ramírez, A. C. R. (Ekstern), González, A. (Ekstern)
Pages: 850-855
Publication date: 2012
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Chemosphere
Volume: 89
Issue number: 7
ISSN (Print): 0045-6535
Ratings:
- BFI (2017): BFI-level 2
- BFI (2016): BFI-level 2
- Scopus rating (2016): SJR 1.417 SNIP 1.606
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.51 SNIP 1.57
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.593 SNIP 1.651
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.724 SNIP 1.767
- ISI indexed (2013): ISI indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.818 SNIP 1.623
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.961 SNIP 1.515
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.867 SNIP 1.421
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.836 SNIP 1.573
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.651 SNIP 1.591
- Scopus rating (2007): SJR 1.511 SNIP 1.616
- Scopus rating (2006): SJR 1.416 SNIP 1.676
- Scopus rating (2005): SJR 1.478 SNIP 1.563
- Scopus rating (2004): SJR 1.633 SNIP 1.494
- Scopus rating (2003): SJR 1.324 SNIP 1.324
- Scopus rating (2002): SJR 0.912 SNIP 1.066
- Scopus rating (2001): SJR 0.928 SNIP 0.975
- Scopus rating (2000): SJR 0.876 SNIP 0.876
- Scopus rating (1999): SJR 1.048 SNIP 0.846
Original language: English
DOIs:
Dynamic multicrop model to characterize impacts of pesticides in food

A new dynamic plant uptake model is presented to characterize health impacts of pesticides applied to food crops, based on a flexible set of interconnected compartments. We assess six crops covering a large fraction of the worldwide consumption. Model estimates correspond well with observed pesticide residues for 12 substance-crop combinations, showing residual errors between a factor 1.5 and 19. Human intake fractions, effect and characterization factors are provided for use in life cycle impact assessment for 726 substance-crop combinations and different application times. Intake fractions typically range from 102 to 108 kg intake kg applied-1. Human health impacts vary up to 9 orders of magnitude between crops and 10 orders of magnitude between pesticides, stressing the importance of considering interactions between specific crop-environments and pesticides. Time between application and harvest, degradation half-life in plants and residence time in soil are driving the evolution of pesticide masses. We demonstrate that toxicity potentials can be reduced up to 99% by defining adequate pesticide substitutions. Overall, leafy vegetables only contribute to 2% of the vegetal consumption, but due to later application times and higher intake fractions may nevertheless lead to impacts comparable or even higher than via the larger amount of ingested cereals.

General information
State: Published
Organisations: Technical University of Denmark, Swiss Federal Institute of Technology, Institute of Agriculture and Food Research and Technology, University of Stuttgart, University of Michigan
Authors: Fantke, P. (Intern), Juraske, R. (Ekstern), Anton, A. (Ekstern), Friedrich, R. (Ekstern), Jolliet, O. (Ekstern)
Pages: 8842–8849
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Journal: Environmental Science & Technology (Washington)
Volume: 45
ISSN (Print): 0013-936X
Ratings:
BFI (2017): BFI-level 2
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 2.538 SNIP 1.889
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.584 SNIP 1.828
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.777 SNIP 2.017
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.956 SNIP 2.103
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.146 SNIP 2.056
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.178 SNIP 1.953
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.964 SNIP 1.729
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.835 SNIP 1.803
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.943 SNIP 1.942
Scopus rating (2007): SJR 2.8 SNIP 1.927
Scopus rating (2006): SJR 2.541 SNIP 1.901
Scopus rating (2005): SJR 2.604 SNIP 2.014
Scopus rating (2004): SJR 2.863 SNIP 2.046
Plant uptake of pesticides and human health: Dynamic modeling of residues in wheat and ingestion intake

Human intake of pesticide residues from consumption of processed food plays an important role for evaluating current agricultural practice. We take advantage of latest developments in crop-specific plant uptake modeling and propose an innovative dynamic model to estimate pesticide residues in the wheat-environment system, dynamiCROP. We used this model to analyze uptake and translocation of pesticides in wheat after foliar spray application and subsequent intake fractions by humans. Based on the evolution of residues in edible parts of harvested wheat we predict that between 22 mg and 2.1 g per kg applied pesticide are taken in by humans via consumption of processed wheat products. Model results were compared with experimentally derived concentrations in wheat ears and with estimated intake via inhalation and ingestion caused by indirect emissions, i.e., the amount lost to the environment during pesticide application. Modeled and measured concentrations in wheat fitted very well and deviate from less than a factor 1.5 for chlorothalonil to a maximum factor 3 for tebuconazole. Main aspects influencing pesticide fate behavior are degradation half-life in plant and time between pesticide application and crop harvest, leading to variations in harvest fraction of at least three orders of magnitude. Food processing may further reduce residues by approximately 63%. Intake fractions from residues in sprayed wheat were up to four orders of magnitude higher than intake fractions estimated from indirect emissions, thereby demonstrating the importance of exposure from consumption of food crops after direct pesticide treatment. © 2011 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Technical University of Denmark, Agroscope, École Polytechnique Fédérale de Lausanne, University of Stuttgart, University of Michigan
Authors: Fantke, P. (Intern), Charles, R. (Ekstern), de Alencastro, L. F. (Ekstern), Friedrich, R. (Ekstern), Jolliet, O. (Ekstern)
Pages: 1639–1647
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemosphere
Volume: 85
ISSN (Print): 0045-6535
Ratings:
BFI (2017): BFI-level 2
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 1.417 SNIP 1.606
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.51 SNIP 1.57
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.593 SNIP 1.651
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.724 SNIP 1.767
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.818 SNIP 1.623
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.961 SNIP 1.515
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.867 SNIP 1.421
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.836 SNIP 1.573
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.651 SNIP 1.591
Scopus rating (2007): SJR 1.511 SNIP 1.616
Scopus rating (2006): SJR 1.416 SNIP 1.676
Scopus rating (2005): SJR 1.478 SNIP 1.563
Scopus rating (2004): SJR 1.633 SNIP 1.494
Scopus rating (2003): SJR 1.324 SNIP 1.324
Scopus rating (2002): SJR 0.912 SNIP 1.066
Scopus rating (2001): SJR 0.928 SNIP 0.975
Scopus rating (2000): SJR 0.876 SNIP 0.876
Scopus rating (1999): SJR 1.048 SNIP 0.846
Original language: English
DOI:
10.1016/j.chemosphere.2011.08.030
Source: dtu
Source-ID: u::5271
Publication: Research - peer-review › Journal article – Annual report year: 2012

Projects:

Addressing inorganic chemicals in life cycle impact assessment
Department of Management Engineering
Period: 15/12/2015 → 14/12/2018
Number of participants: 3
Phd Student:
Müller, Nienke (Intern)
Supervisor:
Hauschild, Michael Zwicky (Intern)
Main Supervisor:
Fantke, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Assessing Life Cycle Impacts of Bio-plastics from Dicarboxylic Acids
Novo Nordisk Foundation Center for Biosustainability
Applied Metabolic Engineering
Quantitative Sustainability Assessment
Department of Management Engineering
Period: 01/11/2015 → 30/11/2018
Number of participants: 4
Phd Student:
Ögmundarson, Ólafur (Intern)
Supervisor:
Fantke, Peter (Intern)
Fürster, Jochen (Intern)
Olsen, Stig Irving (Intern)

Project
Assessing Life Cycle Impacts of Bioplastics from Dicarboxylic Acids

Department of Management Engineering
Period: 01/10/2015 → 30/09/2018
Number of participants: 3
Phd Student:
Ögmundarson, Ólafur (Intern)
Supervisor:
Herrgard, Markus (Intern)
Main Supervisor:
Fantke, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

QUAN-TOX
QUAN-TOX is a four-year project aiming at extending, disseminating, and harmonizing the QUANtification of human and ecosystem TOXicity impacts when assessing the sustainability of products and services over their life cycle. Research will identify and address existing gaps in current toxicity assessment models. Dissemination of research results includes scientific publications and knowledge transfer including teaching activities and elaborating training material. As a result, QUAN-TOX promotes sustainability aspects towards integration into European legislation and strengthens Europe's role in raising scientific awareness of aspects around risk minimization, product optimization, and life cycle thinking, which is in line with the Europe 2020 economy growth strategy. Thereby, QUAN-TOX will play a key role at the interface between researchers in life cycle toxicity assessment and stakeholders including policy makers at the European scale, community organisations, industry, academy, schools and students, and the general public. Finally, QUAN-TOX helps to tackle societal challenges like human health and well-being, sustainable agriculture, and clean energy that all reflect policy priorities according to the Horizon 2020 EU Framework Programme for Research and Innovation.

Department of Management Engineering
Quantitative Sustainability Assessment
Period: 01/04/2014 → 31/03/2018
Number of participants: 1
Ecotoxicity, Human toxicology, Impact assessment, Sustainability
Acronym: QUAN-TOX
Project Coordinator:
Fantke, Peter (Intern)

Project

Quantifying the Sustainability of Consumer Products: Focusing on Chemical Exposures

Department of Management Engineering
Period: 15/12/2013 → 23/03/2017
Number of participants: 9
Phd Student:
Ernstoff, Alexi (Intern)
Supervisor:
Hauschild, Michael Zwicky (Intern)
Jolliet, Olivier (Ekstern)
Rosenbaum, Ralph K. (Intern)
Trier, Xenia (Intern)
Main Supervisor:
Fantke, Peter (Intern)
Examiner:
Olsen, Stig Irving (Intern)
Egeghy, Peter Paul (Ekstern)
Hellweg, Stefanie (Ekstern)

Financing sources
TOX-TRAIN: The implementation of a TOXicity assessment Tool for pRACTical evaluation of life-cycle Impacts of technologies

TOX-TRAIN is a 4-year project and its main objective is the development and implementation of a tool box to assess toxicological impacts related to the life-cycle of technologies. The USEtox model, developed under UNEP-SETAC auspices with contributions of the partners in this consortium, will be taken as a starting point. First, TOX-TRAIN will develop and implement estimation tools for emissions and chemical properties to USEtox for a number of compound groups, including ionic and amphiphilic substances, persistent bioaccumulating chemicals or metabolites, pesticides and biocides, substituted musks/fragrances, and metals, with a specific focus on assessing various types of uncertainty in emissions and properties. The compound groups are selected on the basis of use volumes, fate pattern complexity and main emission route relevance. The tools will be developed as open-source software. Second, the USEtox model will be extended with an indoor compartment model for typical exposure situations in working place and household settings as well as direct consumer exposure through a product (e.g. a directly applied cosmetic product). Third, a number of case studies will be performed in close collaboration between the commercial and non-commercial partners of TOX-TRAIN to test the USEtox tool box in practice. Finally, dissemination of the tool box will be done by a portfolio of actions, such as workshops, course developments, training of specific user groups, documentation material, and a user-friendly web-based implementation. In short, TOX-TRAIN will provide an excellent platform to enhance the transfer of knowledge between the commercial and non-commercial sector in the area of toxic life-cycle impact assessment of technologies. It is envisaged that the developed USEtox tool box has a great market potential as it can be directly used in the daily practice of life cycle assessment studies.

Department of Management Engineering
Quantitative Sustainability Assessment
Quantis
Radboud Universiteit
Veolia Environnement
Period: 01/11/2011 → 31/10/2015
Number of participants: 3
Modelling (Environmental risks), Life Cycle Impact Assessment, Chemical emission-fate-exposure-effects modelling, Intake Fraction, Indoor emissions/exposure, USEtox model, Consumer/Worker exposure
Acronym: TOX-TRAIN
Project participant: Birkved, Morten (Intern)
Ernstoff, Alexi (Intern)
Project Coordinator: Fantke, Peter (Intern)

Relations
Activities: Towards consensus about the delimitation between life cycle inventory and impact assessment in LCAs with pesticide and fertilizer use

LC-IMPACT: Development and application of environmental Life Cycle Impact assessment Methods for imProved sustainAinability Characterisation of Technologies

Department of Management Engineering
Quantitative Sustainability Assessment
Radboud Universiteit
Swiss Federal Institute of Technology
Swedish Institute for Food and Biotechnology
PRé Consultants B.V.
International Institute for Applied Systems Analysis
Unilever
University of Stuttgart
Quantis
Leiden University
European Commission - Joint Research Center
Institute of Agri-food Research and Technology
University of Bayreuth
Period: 01/12/2009 → 31/05/2013
Number of participants: 6
LCA
Acronym: LC-IMPACT
Project participant:
Hauschild, Michael Zwicky (Intern)
Rosenbaum, Ralph K. (Intern)
Larsen, Henrik Fred (Intern)
Fantke, Peter (Intern)
Owsianiak, Mikolaj (Intern)
Cosme, Nuno Miguel Dias (Intern)

Relations
Parent project:
Development and application of environmental Life Cycle Impact assessment Methods for improved sustainability
Characterisation of Technologies
Project

Activities:

**Indicators, frameworks, and instruments to evaluate impacts and costs of chemicals in articles in the circular economy**
Period: 1 Dec 2016 → 2 Dec 2016
Peter Fantke (Invited speaker)
Department of Management Engineering
Quantitative Sustainability Assessment
Documents:
Fantke_2016n.pdf

Related event
**European Environment Agency (EEA) Expert Workshop on Groups of Chemicals in the Circular Economy**
01/12/2016 → 02/12/2016
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**Indoor Chemistry Modeling in Context: What questions do we answer?**
Period: 7 Nov 2016 → 8 Nov 2016
Peter Fantke (Lecturer)
Department of Management Engineering
Quantitative Sustainability Assessment

Related event
**Workshop on Indoor Chemistry Models**
07/11/2016 → 08/11/2016
Washington, United States
Activity: Talks and presentations › Conference presentations