

## Towards a Life Cycle Based Chemical Alternative Assessment (LCAA)

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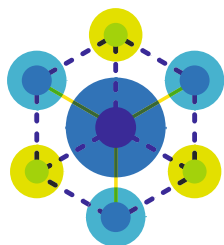
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Increasingly, various stakeholders require information on eco/toxicity aspects of products beyond regulatory requirements for chemicals, e.g. in the framework of Life Cycle Assessment ("LCA"). The method developed (here referred to as "ProScale") aims to be a science-based, transparent, pragmatic and generally applicable methodology for a toxicological assessment of products. It is a development of initial ideas of an approach for merging applicable information from REACH with LCA. The ProScale method has been developed in an industrial consortium with expertise both from the Life cycle assessment and Risk assessment areas. Prerequisites for the method have been to: (i) assess the relevant direct exposure potential along the whole life cycle; (ii) use existing data, e.g. REACH based; (iii) allow comparison in relation to technical performance; and (iv) be relevant for business-to-business and business-to-customer communication. The ProScale method estimates a score for a specific instance of *exposure* for each substance for a given process and exposure route expressed in an Exposure Factor (EF). The EF is modelled based on the ECETOC Targeted Risk Assessment Tier 1 approach for both worker and consumer exposure. This is combined with its corresponding *hazard* for the substance considered expressed in a ProScale Hazard Factor (HF). The HF reflects the health hazard effect severity and potency based on Hazard statement Code(s) (H-phrases) and Occupational Exposure Limits (OEL). Then it relates this score to the amount of different substances in relation to the defined unit process at hand. Subsequently, the method accounts for the amount of each unit process necessary for the fulfilment of the functional unit as defined by the product system/flow chart. This is done for all included exposure instances, so that eventually a large number of ProScale scores for all included exposure instances are making up the ProScale toxicity impact potential for the overall product system of the studied product (PSP = ProScale of Product). A product can in this context also mean a service provided by the system. The smethod structure allows for comparisons based on the same function as for other LC indicators. Currently the basic structure is in place, and case studies are carried out and under way to demonstrate the applicability of the method.

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#### **Learnings from LCA-based methods: should chemicals in food packaging be a priority focus to protect human health?**

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Given the scale and variety of human health damage (HHD) caused by food systems, prioritization methods are urgently needed. In this study HHD is estimated for case studies on red meat and sugary sweetened beverages (SSB) packaged in high-impact polystyrene (HIPS) due to various relevant health impacts.

Specifically, we aim to assess if chemicals in food packaging are important to HHD in a life cycle context. The functional unit is "daily consumption of a packaged food per person in the United States." Method developments focus on human toxicity characterization of chemicals migrating from packaging into food. Chemicals and their concentrations in HIPS were identified from regulatory lists. A new high-throughput model estimated migration into food, depending on properties of chemicals, packaging, food, and scenario, and HHD was extrapolated following LCA characterization methods. An LCA-based study on the packaged foods estimated HHD from particulate matter and chemical emissions. Finally, the HHD of consumption of red meat and SSB above the minimum risk level was estimated using novel methods by Stylianou et al. 2016 based on the Global Burden of Disease studies. Results indicate that impacts caused by consumption of food items over minimum risk are high priority for mitigating HHD, as well as associated PM<sub>2.5</sub> emissions from agriculture. Impacts due to the chemicals migrating from HIPS into food were minor given the study's assumptions, limitations, and methods. However, calculating the HHD for migration levels at the legally allowable limits resulted in impacts three orders of magnitude greater than impacts from the assumed chemical concentrations, and thus a relevant contributor to HHD. Future work is required to quantify realistic exposure to chemicals in packaging and their potential effects in order to elucidate significance in a life cycle context. Understanding toxicity risks posed by simultaneous exposure to several chemicals at one time, all of which are below safety thresholds, requires cross-fertilization with risk and toxicity research. Lastly, the methods developed are a first step towards operationalizing LCA for practitioners to ensure that minimizing impacts on the environment and resources due to food packaging design choices do not lead to unintended health risks caused by chemicals in packaging, and vice versa that minimizing exposure to hazardous chemicals do not increase environmental damages.

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#### **Modeling indoor occupational air emissions of nanomaterials for life-cycle assessment**

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Engineered nanomaterials (ENM) provide industrial and commercial benefits across many sectors but they also raise concerns over their potential environmental and human health hazards. While the technologies that utilize ENM can be evaluated by life-cycle assessment (LCA) to determine their potential resource efficiencies, existing methodologies do not allow for the evaluation of the environmental and human health hazards posed by the emission of individual ENM. Across the life-cycle of nanotechnologies, occupational settings present scenarios where production of pristine particles with small size distributions and thus exposure may occur. Neglecting such occupational, indoor ENM emissions in a LCA may result in burden shifting from the environment to workers. Currently existing life-cycle impact assessment methods take advantage of several assumptions that conveniently describe the fate and transport of small organic molecules and metals quite well, but these methods are not appropriate for ENM. In this paper, a two-zone, *dynamic* fate and transport model is presented for use with indoor, occupational ENM airborne emissions. The fate and transport model is linked to a physiologically-based pharmacokinetic (PBPK) inhalation exposure model that considers the deposition, removal and retention of particles in the lung over time. During emission events, the fate and transport of titanium dioxide nanoparticles resulted in a distinct near-field concentration that was generally twice the concentration of the far-field. During times without ongoing emissions, the near- and far-field concentrations were equal and decreased in-step (i.e. effectively becoming a one-box model when there were no ongoing emissions). Results of a steady-state model show that near-field concentrations were underestimated by roughly 90% of the maximum concentrations calculated using the dynamic model in this abstract. Inhalation exposure and final retention of particles in the lung was significantly influenced by the magnitude of the airborne concentration. As airborne concentrations rose significantly, phagocitizing cells in the air-exchange and interstitial regions became saturated. The results of the fate and exposure model were compared with a number of emission scenarios ranging from low to medium to high emission events. A notable finding was that the retained-intake fraction was inversely related to the emission magnitudes, which is counter-intuitive to conventional thinking in LCA.

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#### **Towards a Life Cycle Based Chemical Alternative Assessment (LCAA)**

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There is a need for an operational quantitative screening-level assessment of alternatives, that is life-cycle based and able to serve both Life cycle Assessment (LCA and chemical alternatives assessment (CAA). This presentation therefore aims to develop and illustrate a new approach called "Life Cycle Based Chemical Alternative Assessment (LCAA)" that will quantify exposure and life cycle impacts consistently and efficiently over the main life cycle stages. The new LCAA approach is illustrated through a proof-of-concept case study of alternative plasticizers in vinyl flooring. The proposed LCAA approach combines the following elements: a) The manufacturing phase chemical inventory is based on the environmental genome of industrial products database, ensuring mass and energy balance, b) near-field exposure to consumer products during the use phase is determined based on the mass of chemical ingredient in the product, first-order inter-compartmental transfer fractions and a matrix approach to determine Product Intake Fractions, and c) toxicity-related outcomes are compared with other life cycle impacts to evaluate the relevance of different impact categories for different consumer product classes. The retained case study is a comparison of two alternative plasticizers (DEHP-diethylhexyl phthalate vs. DIHP-Diisooheptyl phthalate) in vinyl flooring. First order release rates of DEHP and DIHP from flooring material to indoor air are restricted, with over the first three years a maximum of 0.4% of the SVOC initial content in flooring emitted for DEHP and 1.9% for DIHP. For climate change, there is little difference between the two plasticizers, whereas compared to DEHP, DIHP impacts are reduced by a factor 10 for human health and a factor 3 for ecotoxicity. This proof of concept case study demonstrates the feasibility of combining chemical specific Life Cycle Inventory from manufacturing database with near-field exposure assessment during product use and to compare the interest of various chemical alternatives. Considering consumer exposure during use phase is essential for both LCA and ACC, the determination of Product Intake Fractions using first order transfer matrices enabling a parsimonious exposure assessment.

#### **Environmental risk assessment of biocides: regulatory requirements, challenges and consequences**