Near-field exposure factor modeling of chemicals in personal care products

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14:15 *Olivier Jolliet*, *Peter Fantke*, *Lei Huang* and *Alexi Ernstoff*
Accounting for near-field exposure to chemicals in consumer products in LCA
SPEAKER: *Olivier Jolliet*

ABSTRACT. Every consumer product has the potential to expose humans to chemical ingredients during use, via multiple exposure pathways. However, many product oriented exposure assessment accounts mostly for indirect environmental exposure and not direct exposure of consumer to product during use. We therefore aim to a) Identify the most efficient interface between LCI and LCIA for the use and disposal stage of consumer products, b) determine the chemical concentration in product as an LCI input, c) define and calculate the Product Intake Fraction (PiF), a metric that accounts for near field exposure in LCA:, d) demonstrate the framework and models through examples from various consumer products. We propose to first determine the mass of chemical in product per functional unit (FU) as inventory flow and point of departure to then calculate intake and impact. This inventory flow is the amount of product used per FU multiplied by the chemical content in product. This content is either based on measured data, derived from household product databases, or determined based on chemical -product specific function and frame formulations. Intakes are then determined using the product intake fractions - the fraction of the chemical in product that is taken in via each exposure pathway, considering the specific point of entry (cosmetics, chemical in article, indoor air, etc.). We propose a new near & far field multi-media matrix of transfer fractions, with one column and row for each point of entry, for each environmental compartment and for each exposure pathway. The multiple transfer and product intake fraction (e.g from chemical in article to inhalation of indoor air) is obtained by inverting the transfer fraction matrix, yielding the infinite multi-media transfer fractions. Product intake fraction range from 10e-7 for an SVOC in a thick flooring, to 5e-3 for an indoor air emission up to 96% for a leave-on cosmetic ingredient.

14:30 *Susan A. Csiszar*, *Alexi S. Ernstoff*, *Peter Fantke*, *Olivier Jolliet*, *Jane Bare* and *David Meyer*
Near-field exposure factor modeling of chemicals in personal care products
SPEAKER: *Susan A. Csiszar*

ABSTRACT. It has been estimated that there are thousands of chemicals used in personal care products (PCPs) and human exposure to these

chemicals can be dominated by the use stage. Within chemically mediated human health (HH) life cycle impact assessment (LCIA), focus has historically been on far-field environmentally mediated exposures with less focus on exposure occurring in the near-field (e.g. in the indoor environment) during the product use stage. We used the concept of the product intake fraction (PiF) [1] to estimate near- and far-field exposure factors associated with chemicals in PCPs. We combine these with effect factors available in USEtox [2] to calculate characterization factors (CFs) for a subset of PCP chemicals and compare them to CFs associated with far-field emissions.

The PiF can be used to quantify the amount of chemical taken in per mass of chemical used in a PCP and can be combined with product composition to estimate chemical intake due to product use. The use-stage PiF for PCPs was estimated using mass balance modeling with physicochemical properties and product usage characteristics (e.g., leave-on or wash-off) as data inputs for dermal aqueous uptake, gaseous dermal exposure, and inhalation. Disposal stage PiFs were estimated by combining the fraction of chemical washed down the drain after product use and USEtox calculated far-field intake fractions. Additionally, to understand which physicochemical properties drive use-stage exposure, we calculated PiFs for a range of properties.

Varying physicochemical properties indicates the PiF is dominated by dermal aqueous uptake when a chemical has a relatively large Kow (octanol-air partition coefficient) combined with a relatively small Kaw (air-water partition coefficient). Furthermore, use-stage PiFs were 4-100% and 0.001-100% for leave-on and wash-off products, respectively, indicating a variability of about five orders of magnitude across PCP chemicals. Disposal-stage PiFs were 0-0.3% and in general were several orders of magnitude smaller than use-stage PiFs, however, some chemicals had comparable use- and disposal- stage PiFs. CFs for PCP use thus may have substantially different ranking compared to CFs for far-field releases and may dominate overall impact scores.

1. Jolliet et al., 2015, Environmental Science & Technology, Submitted. 2. http://www.usetox.org/

14:45 *Yuan Yao*, *Diane Graziano*, *Matthew Riddle* and *Eric Masanet*
A Case Study of MAMTech Assessment Model: Prospective Life-cycle Technology Assessment of Future U.S. Ethylene Production
SPEAKER: *Yuan Yao*

ABSTRACT. MAMTech (Macro-level Technology Assessment Model) is a modeling framework integrating chemical process design and modeling, life cycle assessment and techno-economic analysis for assessing the net energy and emissions implications of technology changes in the U.S. chemical production from a life cycle perspective. This assessment is critical because it can provide policy makers with good references on future investment and technology promotion, provide manufacturers and researchers with better understanding on technology potentials, possible bottlenecks and directions for future improvements. However, the assessment of new technology is challenging for lack of process data, general evaluation approach across different products and robust methodology over the temporal scale[1]. MAMTech is designed to overcome these barriers.

In this work, MAMTech is used to evaluate the macro-level life cycle energy and GHG emissions of several emerging technologies for ethylene production; in order to (1) demonstrate the function of MAMTech; (2) provide prospective insights on the energy and emissions reduction potentials of different technologies for ethylene production in future decades. Ethylene is chosen because it is one of the largest energy consumer and GHG emissions resources in chemical industry. According to IEA's analysis, ethylene accounts 13% of global energy consumption and 15% of GHG emissions[2, 3].

Based on the preliminary results, 100-150 million GJ/year of energy consumption can be saved in the U.S. ethylene production life cycle under a high feedstock supply scenario through a new catalysis-based technology for steam cracker. This reduction of energy consumption mitigates 7-18 million ton of CO2-e/year. The ranges given here are based on results of Monto Carlo simulation considering uncertainties and system variances. Regarding the emerging technology that is not for improving current process but an alternative production pathway, MAMTech is able to overcome the knowledge barriers and provide a credible assessment by integrated modules of life cycle assessment and chemical process design. The results of different technologies are later compared together at different scenarios.

The results can shed the light on technology opportunities with the largest reduction potentials of energy and GHG emissions at a foreseeable time frame. The modeling framework itself is an effective tool assisting policy making, environmental and energy analysis, and R&D.

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14:00-15:30 Session 4D: Industry Special Session: Part 1