Fully quantitative, mass-balance-based framework to consistently quantify high-throughput exposure and human toxicity effects for ~10,000 chemicals found in consumer product applications

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This meeting intends to progress towards a broadly accepted framework to assess and position the safety of trace chemicals exposure from consumer products, and in particular from articles and assembled consumer goods.

Program Structure: The scientific program for this workshop is segmented according to each theme. Each presentation will be approximately 20–25 minutes long, and each theme contains a mix of invited speakers and speakers selected from submitted abstracts. Each theme will close with a moderated panel discussion that allows audience members and speakers to engage in productive dialogue to help address central questions related to each theme. Theme 5, "Towards a Risk Assessment Best Practice Framework" is intended as an interactive session that allows for rotating group dialogue among attendees.

In addition to the presentations there will also be poster sessions on Monday and Tuesday evenings. The poster sessions are intended to allow all attendees to present related research and findings, share ideas, and increase collaboration.

Detailed Scientific Program

SESSION: Global Databases for Exposure Information

Fully Quantitative, Mass-Balance-Based Framework to Consistently Quantify High-Throughput Exposure and Human Toxicity Effects for ~10,000 Chemicals Found in Consumer Product Applications

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Evaluating exposure is important to identify viable alternatives to harmful chemicals in products. Yet, current substitution methods lack efficient and flexible approaches to quantify exposure for the numerous product-chemical combinations. To address this gap, we present an operational matrix-based high-throughput framework efficiently coupling multi-pathway near-field (worker and consumer) with far-field (general population) exposures.

We first determine the chemical mass in a product and define the compartments in which chemicals enter the environment, e.g., 'object surface layer' for cleaning products. We then structure fractions transferred to other compartments and humans in a matrix, using seven product models. Inverting this matrix yields cumulative transfer fractions and Product Intake Fractions linking chemical mass taken in by humans to mass of chemicals in products. We finally determine exposure doses or exposures based on product functions. Our framework was applied to generate high-throughput exposure results for 8000+ chemicals in Tox21 and for 9000+ product-chemical combinations commonly used in the US.

Exposure estimates range from 0.7 ppm to 93% across chemicals. Exposure doses for product users can vary from 1E-9 to 400 mg/kgBW/d, dominated by inhalation and dermal exposure. For each product application, we are able to determine the chemical-specific contributions of pathways and population groups to overall exposure and compare relative exposure magnitudes across chemicals in a given product. Combining these exposures with toxicity data, we are able to identify main chemicals of concern and rank alternatives. Systematic sensitivity studies enable us to identify the most important product and chemical attributes and produce heat maps to easily determine exposure, for use in a screening substitution approaches, as will be illustrated for chemical alternatives in several product types. The more detailed mass-balanced-based framework is readily available for use by substitution practitioners to screen a wide range of product-chemical combinations.