A multi-compartmental framework for near and far-field exposure to consumer products

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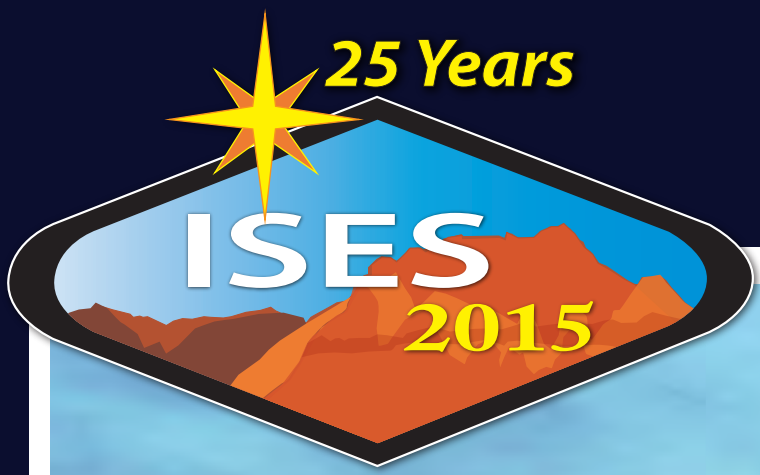

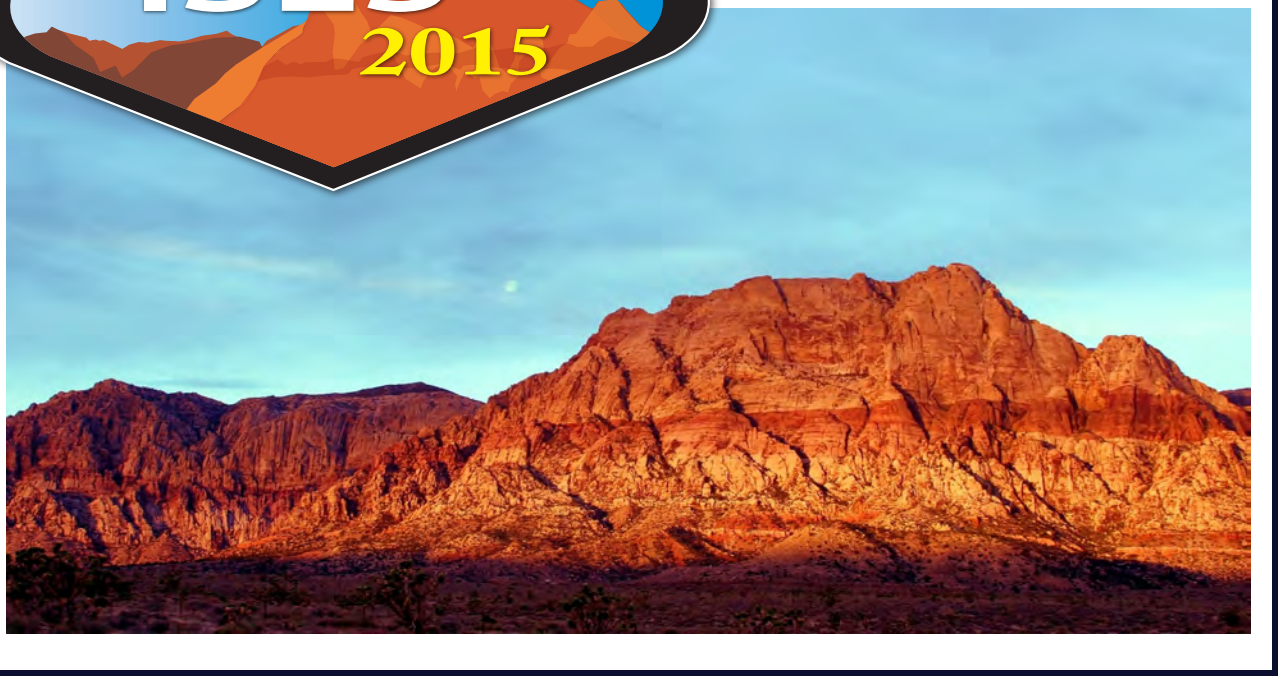

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chemical over consumer product life cycle. Chemicals encapsulated in products can be a major emission source in the use phase. Previous models describing such emissions require complex analytical or numerical solutions, which poses a great computational burden and lack transparency. In the present study, we adapted a model which describes (S)VOC emissions from building materials and subsequent loss by ventilation, and simplified the governing equations by assuming a pseudo-steady-state between emission and loss and introducing a modified convective mass-transfer coefficient (hm'). Results of this simplified model show a good agreement with the original full model and the experimental data. The solution of this simplified model for mass fraction emitted, which consists of a sum of an infinite series, is further reduced to a sum of only two exponentials with parameters which can be predicted from physiochemical properties using explicit equations. Results of this simple two-exponential model agree well with the original full model over 15 years with R-square greater than 0.99 for a wide range of 264 compounds and material thicknesses. Moreover, the chemical concentration at the material surface can be simply calculated from the derivative of this two-exponential model, which also agrees well with the original full model. This parsimonious approach greatly reduces the computational burden, which is suitable for high-throughput screening of chemical emissions and exposure potentials. The inhalation and dermal exposure doses derived from the mass fraction emitted and surface concentration will then be compared with Oral Equivalency Doses back calculated from ToxCast bioassays.

Keywords: C-consumer products, A-exposure models, encapsulated chemicals, A-indoor environment

Mo-O-G3-02

Tier 2 High-Throughput Exposure Screening of Chemicals in Consumer Products: Chemicals encapsulated in articles and in cosmetics

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Abstract: The ExpoDat initiative has developed a Tier 1 high throughput risk screening framework based on Total Production Volumes, showing that a fraction of screened chemicals may have exposure estimates exceeding in vitro bioactivity. There is a need to develop a Tier 2 framework based on effective chemical concentrations in products to refine models and improve exposure estimates. The proposed ExpoDat Tier 2 framework involves four steps: a) Chemical product-use identification, b) collection of usage data and chemical concentration ranges, e.g. based on chemical function and frame formulation guides, c) refined modeling of Product Intake Fraction (chemical mass taken in per kg in product) and intake doses in mg/kg/day, and d) model evaluation and comparison with ToxCast derived Oral Equivalency Doses (OEDs). The Tier 2 framework is tested in priority for pathways and use scenario modules with strong potential for improvement, i.e. cosmetic ingredients as a direct pathway and chemicals encapsulated in objects for passive releases. For cosmetics, intake doses may exceed 1 mg/kg/d by more than a factor 10 for a high end user of leave-on products and a high chemical content. This may thus also exceed some of the corresponding OEDs by orders of magnitude. When exact chemical content is unknown, but chemical function is known, it is possible to use frame formulations to define plausible ranges in chemical content for a given function-product combination (e.g. for solvent in body lotion). For chemicals encapsulated in flooring materials, intake doses are lower, from 10e-5 to 10e-1 mg/kg/d. Doses increase with initial chemical content (high for SVOCs plasticizers) and with fast release kinetics (fastest release for VOCs). For such chemicals in articles, exact chemical content and formulations are often unknown and the developed model may be used to back calculate maximum chemical content of e.g. 0.1% for phenol in flooring, that corresponds to a potentially bio-active intake dose.

Keywords: A-chemical prioritization, A-exposure models, A-risk assessment, C-consumer/personal care products, C-consumer products

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A multi-compartmental framework for near and far-field exposure to consumer products

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Abstract: Every consumer product has the potential to expose humans to chemical ingredients during use, via multiple exposure pathways. To quantify these exposures in a consistent way, we first need to address two challenges: a) How should data on chemical, function, chemical-product combination and point of entry in the near and far field environment be structured and combined in a systematic way? b) How to link the different

points of entry in the near and far field environment in a multi-media framework to calculate product intake fractions - the fraction of the chemical in product that is taken in via each exposure pathway, while considering the specific point of entry (cosmetics, chemical in article, indoor air, etc.), product characteristics and chemical properties? We first combine quantitative information on chemical content in consumer products per in-product functional use and on product use with qualitative information on chemical classes to link chemicals to chemical functions and products, to link products further to points of entry and to finally estimate chemical concentration for each point of entry. We then propose a new near & far field multi-media matrix framework, with one column and row for each point of entry, for each environmental compartment and for each exposure pathway. Using point of entry specific exposure models, we create a matrix of transferred fractions between individual compartments, describing the first order fractions of chemical directly transferred from one compartment to adjacent compartments (e.g. fraction of chemical in article transferred to indoor air) . The multiple transfer and product intake fraction (e.g from chemical in article to inhalation of indoor air) is simply 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.

Keywords: A-exposure models, A-risk assessment, A-life cycle analysis, C-consumer products, Product Intake Fraction

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Comparison of Consumer Exposure Models and Indoor Exposure Pathways

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Abstract: Consumer products and articles can be significant sources of indoor chemical exposures. Products are typically liquids, aerosols, or solids and are consumed and used a given number of times, over time, before they are discarded. Articles are typically solids and are always present within indoor environments for the duration of their useful life. Recent updates to the U.S. Environmental Protection Agency's Consumer Exposure Model (CEM) have increased the scope and versatility of the tool, expanding the exposure pathways and product/article use scenarios that can be assessed. Capabilities of CEM, along with other consumer exposure models, will be compared with refined product and article use categories to assess gaps. There are twelve models included in the beta testing version of CEM which cover inhalation, ingestion, and dermal exposure pathways. This presentation crosswalks all possible indoor exposure pathways with those currently incorporated into consumer exposure models. There are close interrelationships between exposure pathways that will be explored. Additional models that are not yet included are also discussed; these models tend to be reliant on empirical data and estimation approaches which are not well developed. For example, articles that are in contact with and contain chemicals which may migrate into water, products that spill or leak over time, and multi-zone transport of particles within indoor environments over time. Near-term revisions will address comments received during peer review which may include refinements to existing models within CEM or incorporation of new models. Longer-term revisions could continue to incorporate empirical data for model inputs and novel estimation approaches for all indoor exposure pathways. The views of the authors of this abstract are those of the authors and do not represent Agency policy or endorsement.

Keywords: C-consumer products, A-exposure models, C-indoor

Mo-O-G3-05

Integrated Model Framework for Chemical Emissions from the Use of Consumer Products: Human Exposure to Ozone Formation Potential

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Abstract: Background/Aims: Many low vapor pressure-volatile organic compounds (LVP-VOCs) are used in consumer products with down-the-drain applications (e.g., laundry or dishwashing detergents, shampoo, etc.). Depending on whether LVP-VOCs are directly emitted to air in a home during product use or disposed of down the drain, many endpoints of interest, such as human exposure and ozone formation potential, might be widely different. The goal of this study is to develop an integrated model framework to better evaluate the impact of consumer product LVP-VOCs on human exposure and ozone formation potential. Methods: For the fraction that volatilizes to air in a home during use, we applied an indoor exposure model to calculate intake fractions (iF), the integrated cumulative intake of a chemical per unit of emission, and also applied an outdoor multimedia