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## Prioritizing consumer product categories based on exposure estimates

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the toluene exposure indoors to the total life cycle impact of a magazine (44%), we demonstrated that the indoor compartment requires particular attention and that RA and LCA results provide complementary information.

#### **215 Volatile Chlorinated Solvents from Consumer Products:**

**Emissions to Exposures** W.J. Doucette, T. Wetzel, Utah State University / Utah Water Research Laboratory; E. Dettenmaier, K. Gorder, Hill Air Force Base. Volatile organic compounds (VOCs), including many with documented short- and long-term adverse health effects, can enter indoor environments through internal (i.e. consumer products, building materials) and external sources (i.e. vapor intrusion from contaminated groundwater). Indoor air concentrations of VOCs vary widely, but concentrations of most VOCs are consistently higher indoors than outdoors. Many consumer products such as adhesives and cleaning solvents contain volatile chlorinated organic compounds (cVOCs) such as trichloroethene (TCE) tetrachloroethene (PCE) that are also the focus of soil and groundwater cleanups in the USA and Europe. In this study, emissions rates of volatile chlorinated solvents from several consumer products (opened and unopened) including adhesives (PCE), cleaning solvents (TCE), household cleaning products (CCl<sub>4</sub>) and molded plastic objects (1,2-DCA) were measured using a flow<sup>4</sup> through laboratory chamber approach. Measured emission rates varied from 0.001 to 20 ug/min depending on the product and CVOC. Subsequent screening-level calculations suggested that the emissions from some these items could lead to indoor concentrations high enough to be of regulatory concern. To verify this, several controlled release experiments were conducted in an actual residence. Consumer products were introduced into a single room of the test residence and indoor air concentrations of CVOCs were measured throughout the house over time using sorbent tube sampling followed by thermal desorption gas chromatography/mass spectrometry (GC/MS) and/or a portable GC/MS. Measured indoor air concentrations of PCE and TCE peaked within the "source" room and became relatively uniform throughout the residence within several hours after being circulated through the heating, ventilation, and air conditioning (HVAC) system. Both opened and unopened consumer products emitted significant amounts of chlorinated solvents that could confound VI investigations. Initial indoor air concentrations of chlorinated solvents were highest in the room where the consumer products were introduced but were quickly and uniformly distributed throughout the three level house when circulated with the HVAC system. The measured emission rates could be used along with a simple box model to estimate exposure concentrations after "mixing" with the HVAC system.

#### **216 The Fate of PBDEs in The Use and Waste Phases Following Changes of PBDE Levels in Products; An SFA Application**

A. Golnosh, University of Toronto / Geography; A. Buser, ETH Zurich; M.L. Diamond, University of Toronto / Department of Earth Sciences. Brominated flame retardants (BFRs) are synthetic additives which are widely used to reduce the flammability in consumer products. Due to their persistent, bioaccumulative and toxic (PBT) properties, some representative of BFRs such as polybrominated diphenyl ethers (PBDEs) were regulated or phased out in Europe and North America. Despite the global decline in the use of PBDEs, the large inventory of flame retarded products will continue to contribute to emissions of these compounds into indoor and then outdoor environments. Further, "old" PBDEs may return in new consumer products fabricated with recycled materials. In this study, a substance flow analysis (SFA) was used to characterize the flow of PBDEs from product inventory to the surrounding environment. This system is built upon a detailed dynamic inventory of flame retardant products for North America (US and Canada). The results show the changing PBDE inventory over time in the use and waste phases as a result of changes in PBDE levels in consumer products. The outcome of this study can be served as a rational basis for planning systematic action and measures to reduce of the use and human exposure to these substances.

#### **217 Evaluation of the Stockholm Multimedia URban Fate (SMURF)**

**model – application to BDE 209 and two phthalate esters** A.P. Palm Cousins, Natural Resources and Environmental Effects; T. Holmgren, Umea University / Department of Chemistry; M. Remberger, IVL Swedish Environmental Research Institute / Natural Resources and Environmental Effects. The indoor environment has been proposed to play an important role for release of SVOCs to urban air as a result of emissions from consumer products. Cousins (2012) recently studied the contribution of emissions indoors to outdoor pollution using an indoor-inclusive multimedia fate model (SMURF). The aim of this study was to evaluate the SMURF model using realistic emission estimates and real monitoring data and through uncertainty analysis. The SMURF model is a steady state, 8-compartment multimedia fate model parameterized for the municipality of Stockholm. The model incorporates a novel indoor module representing the indoor environment of Stockholm. Evaluation was conducted using emission estimates of DINP, DEHP and BDE 209 based on data from literature and from new emission tests studying the emissions of DINP from PVC materials. Measurements in urban air and ventilation outlets were performed and used in combination with literature data for comparison with model predicted concentrations. Predicted concentrations agreed well with monitoring data for phthalates, but BDE 209 concentrations were a factor of 100 too low, indicating that current emission estimates for BDE 209 do not capture all the important sources. Emission to indoor air, background concentration and ventilation rate were influential inputs for the variance in the target outputs for all substances. The wet removal rate contributed significantly to the variability in dust concentration. The indoor vertical deposition contributed to the variance in all target outputs for BDE 209, reflecting the capacity of BDE 209 to partition to particles, thus emphasizing that particle behaviour is central for the fate of BDE 209. Cousins, A.P. 2012 The effect of the indoor environment on the fate of organic chemicals in the urban landscape. Science of The Total Environment. 438(0): p. 233-241.

#### **218 Prioritizing consumer product categories based on exposure estimates**

A. Ernstoff, School of Public Health, University of Michigan; P. Fantke, Technical University of Denmark; O. Jolliet, University of Michigan / School of Public Health. Data on exposure to consumer products and the chemicals therein is limited and costly to obtain. To prioritize mitigation efforts on chemicals and consumer product categories of concern, we must systematically predict dominant consumer product exposure pathways for a range of chemicals even when empirical data are absent. In this study we present a risk assessment framework for modeling cumulative exposure to consumer products with the end goal of identifying the contribution of each exposure pathway. We investigate a case study of parabens (methyl-, ethyl-, butyl-, and propyl-) in dermally applied cosmetics. Dermal exposure to cosmetics is often not considered in risk assessment and evaluation of cumulative exposure with respect to population scale *in vivo* chemical concentrations. To validate our predictions of consumer exposure we compare modeled results with *in vivo* US National Health and Nutrition Examination Survey NHANES data, and provide insight to develop a consistent and accurate evaluation of chemical exposures through various consumer product uses. Results suggest our method may aid predicting consumer exposure (specifically the 95%-ile of consumer exposure for women) to chemicals, like parabens, found in cosmetics. Estimated doses for daily use range from 0.001 to 0.04 mg/kg/day, and urine loads, extrapolated from NHANES *in vivo* data, are at comparable magnitude. Paraben-specific predicted doses correlate best with NHANES 95%-ile for women especially when considering the maximum likely concentration of each respective paraben ( $R^2=0.60$ ). Most importantly, predicted doses best correlate with urinary loads (95%-ile for women) when adjusting the dose by the relative occurrence in paraben-containing cosmetics ( $R^2=0.97$ ) across ranges of likely concentrations within the products. Using an advanced skin permeability model to estimate systemic absorption through skin does not improve prediction of urinary excretion. As parabens are also present in some foods, oral exposure must also be considered; however, is likely negligible in comparison to dermal exposure to cosmetics. Urinary doses of CP-related chemicals are orders of magnitude higher than exposure to

many environmental contaminants, this considered with our findings suggests dermal exposure to cosmetics is an exposure route category which must be prioritized within the overall framework for calculating human exposure to chemicals in consumer products.

**219 Comparison of generic modelling of emissions from different material sources** T. Holmgren, Umea University / National CBRN Defence Centre; P. Andersson, Umea University; P. Haglund, Department of Chemistry. Building materials and consumer goods contain organic additives that may be released to indoor air and reach the environment. In this study, 2 generic models were developed and compared with experimental data. Three cases were studied: emissions of di-isobutyl phthalate (DIBP) from vinyl flooring to air, triphenyl phosphite (TPP) from LCD-TVs to air, and leaching of triisobutyl phosphate (TiBP) and tributyl phosphate (TBP) from concrete to water. Emissions to air were studied using a 1 m<sup>3</sup> emission chamber. Four vinyl floors and a 32-inch LCD-TV were tested; the TV at various conditions (standby, on, 40°C, and 60°C). Exhaust air was sampled on PUFs for 10 days, test object removed, and chamber heated to recover residues. Concrete leaching tests were made using 9 concrete cylinders, 3 with TiBP, 3 with TBP, and 3 without additive. Water was circulated around cylinders for 16 weeks. Samples (daily/weekly) were extracted with hexane and analysed with GC-MS and GC-FPD. The generic model used to predict emissions used an Abraham solubility model to estimate partition, the Piringer equation to predict diffusion and the Chilton–Colburn analogy to estimate convective mass transfer. Emission factors were calculated using a numeric solution and a simplified model that do not consider material diffusion resistance. When additive concentration is high and additive volatility low the depletion of the material surface is insignificant and diffusion in the material of low importance. This was clearly the case for the LCD, Figure 1, in which TPP are added at high concentration to the front layer of the LCD-screen. It was, however, not the case for the vinyl materials for which the simplified model overestimated the emissions. For such thick materials the material resistance to mass transfer had to be considered and the detailed model used. For concrete, the prediction models did not fit experimental data. In hardened cement, capillary pores and cracks are formed that disturbs the cement structure. Experiments showed an initial release of 4200 µg TiBP / m<sup>2</sup>h, which rapidly dropped to 10 µg/m<sup>2</sup> h. The initial release could be explained through a porosity model and the lower long time release through diffusion theory.

**220 An overview on emerging contaminants** J. Readman, .

**221 The integration of chemistry with toxicological testing in European systems** M. Lamoree, Chemistry & Biology.

**222 Effects of multistressors and bioinvasions in estuaries and coastal areas: implications for ecological risk assessment** L. Guilhermino, CIIMAR University of Porto.

**223 Alternative flame retardants in the coastal and marine environment** R. Ebinghaus, Helmholtz-Zentrum Geesthacht.

**224 What Defines Nanomaterials? - An examination of the size dependence of physicochemical properties critical to environmental risk assessment** C.D. Hassinger, ARCADISUS; K. Sellers, ARCADIS; E.A. Bleeker, RIVM; W.J. Peijnenburg, RIVM / Laboratory for Ecological Risk Assessment; D. Sijm, National Institute for Public Health and the Environment (RIVM). Efforts to assess the risks from nanomaterials implicitly incorporate a definition of what it means to be “nano”. Members of the scientific community and regulators around the world commonly use a definition of 1-100 nanometers (nm) in size. However, uncertainties about this definition persist, with some defining nanoparticles as sizes up to 2000 nm. This presentation will describe, based on a comprehensive literature review, what is known about the size dependence of the physical/chemical properties critical to environmental risk assessment (the known knowns) and current data gaps (known unknowns). As the size of a particle decreases into the

‘nano’ size range some physicochemical properties may significantly change. Therefore, within the context of the European Commission’s (EC) definition of “nanomaterial” and the data needs under the Registration, Evaluation, Authorisation and Restriction of Chemical substances (REACH) regulation (EC 1907/2006), this research sought to determine which physicochemical properties make a nanomaterial different from a ‘conventional’ material and at what size these properties are changed to ‘nanospecific’ properties. The literature review focused on: surface morphology, crystalline structure, water solubility, reactivity, and photocatalytic reactivity. Relative few papers were identified investigating size-related changes in surface morphology. With respect to crystallinity, which can affect reactivity, several aspects of metals and metal oxides (e.g., lattice contraction/expansion, phase transformation) may vary with particle size although no simple conclusions can be drawn regarding size dependence. Some experimental data show that the solubility of metal and metal oxides and sulphides can increase at nanoscale; additionally, the increased rate of solubility is well known. Reactivity can also increase with decreasing particle size. Maximum catalytic activity of nanoparticles occurs at sizes well below 100 nm (15-20 nm), with a sharp change in reactivity below approximately 5 nm in some cases. Photocatalytic reactivity of certain metal oxides and sulphides also increases with decreasing particle size, in some cases changing at a particle size of approximately 5-10 nm. These studies reviewed primarily investigated nanoparticles

**225 Mechanistic interpretation of single-particle ICP-MS data** G. Cornelis, University of Gothenburg / Department of Chemistry and Molecular Biology; M. Hasselov, Goteborg University / Chemistry Dept. Progress in (Eco)toxicological research on fate and effects of engineered nanoparticles (ENP) is hampered by a lack of sensitive methods that can measure particle number-based size distributions (PSDs) of ENP in environmental matrices at realistically low concentrations. Single particle inductively coupled plasma mass spectrometry (spICP-MS) is a promising technique in this respect as it offers element specific measurements of ENP that generate ion bursts in the plasma, the magnitude of which corresponds to their size and the number of which corresponds to the frequency of particles, thus allowing to calculate PSDs. However, the lower size limit of ENP size measurements is limited mainly by lack of a process-based data analysis tools. The current study proposes an alternative approach, where precise knowledge of dissolved and background signals in ICP-MS is used to deconvolute it from spICP-MS. Well-characterised gold ENP of 10, 30 and 60 nm were analysed using spICP-MS and the data was analysed using known algorithm and the algorithm proposed in this study. It is proposed that much more accurate PSD can thus be obtained, especially for relatively small ENPs. A mechanistically based spICP-MS signal analysis algorithm was thus developed that was able to deconvolute dissolved signals from ENP signals in a combined dataset, but in the case of small ENP, there was no statistically significant difference between dissolved and ENP signals that could be used to distinguish the signals, effectively imposing a size limit to spICP-MS determinations of PSDs and concentrations of ENP in the environment.

**226 Fate of nanosilver in lake mesocosms** C.D. Metcalfe, L. Furtado, Trent University / Environmental & Resource Studies; J. Fischer; M. Hoque, H. Hintelmann, Trent University; D. Mitrano, J. Ranville, Colorado School of Mines; B. Cheever, M. Xenopoulos, P. Frost, Trent University. Silver nanoparticles (AgNPs) are widely used in textiles and in household products as antimicrobial additives. AgNPs may enter aquatic ecosystems via discharges of municipal and industrial wastewater. AgNPs undergo transformations in aquatic environments that can alter the toxicity to aquatic organisms. In a study conducted as part of the Lake Ecosystem Nanosilver (LENS) project, we studied the transformations and fate of AgNPs in 12 mesocosms (2 m diameter x 2 m deep) installed in a soft water lake in Ontario, Canada. AgNPs with a mean diameter of 50 nm and capped with either PVP or citrate were purchased as a suspension in deionized water from NanoComposix, CA, USA and this material was added to mesocosms either as incremental (“drip”) additions every second day for a 70 day period, or as a single