High Throughput Modeling of Indoor Exposures to Chemicals

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Risk due to chemical exposure is a function of both chemical hazard and exposure. Proximate sources of exposure due to the presence of a chemical in consumer products (i.e. near-field exposure) are identified as key drivers of exposure and yet are not well quantified or understood. The ExpoCast project is developing a model that forecasts indoor exposure to chemicals used as additives in textiles. Flame retardant chemicals can be found in flooring, upholstery, and articles of clothing. Depending on their physicochemical properties, they may bio-accumulate in the indoor environment at higher magnitudes than in the outdoor environment, which is correlated with high indoor exposure rates. Halogenated flame retardants, such as polybrominated diphenyl ethers (PBDEs), are semi-volatile organic compounds (SVOCs) that have been shown to bio-accumulate. PBDEs are potentially harmful to humans in that they may alter thyroid function, particularly at early developmental stages. In this study, ExpoCast predicted emissions of 74 chemicals found in 32 flooring materials for which gas phase concentrations were measured by Wilke *et al.* (2004).[1] Flooring materials include a range of natural and synthetic floor coverings, installations, and adhesives. Emissions calculations principally depend on the gas-phase concentration of the SVOC in the material as well as the surface area of that source.[2] A linear regression yielded R^2 - and p- values of approximately 0.3 and 2.0E-12, respectively, with logP and vapor pressure being the most significant predictors for gas-phase concentration followed by their presence in adhesives and resilient flooring materials. These results potentially allow for the forecasting of gas-phase concentrations of chemicals for which their analytical data in flooring materials are lacking. Data generated from high throughput exposure methods are then combined with high-throughput screening data from the ToxCast project in order to scientifically assess risk in a time and cost effective manner. As a result, comprehensive risk assessment of indoor use chemicals may be achieved that takes into account their physicochemical properties along with the materials that contain them in a near-field mass balance approach. *This abstract does not necessarily reflect EPA policy.*

1. Wilke *et al. Indoor Air* **2004**, *14*, 98-107

2. Little *et al. Environ. Sci. Technol.* **2012**, *46*, 11171-11178