Advancing Exposure Models to Capture a Broad Continuum of Exposure Scenarios

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The overall objective of this project is to develop and evaluate a modeling framework capable of calculating exposures over a continuum of spatial/temporal scales resulting from a broad range of emission types and product uses. To achieve this objective, we are producing a model that is comprehensive, transparent, and can be run quickly for thousands of chemicals. We will integrate the Bennett Indoor Fugacity Model with a nested CalTOX model, allowing users to determine exposures and intake fractions resulting from emissions at different levels of organization (indoor, urban, regional, and global).

In the first year we (1) studied indoor residence times of semivolatile organic compounds (SVOCs) to understand the persistence of chemicals indoors and (2) modified the Bennett Indoor Fugacity Model to calculate intake fractions, the integrated incremental intake of a chemical per unit of emission, for a suite of SVOCs. As residence times of SVOCs are a major and mostly unavailable input for residential exposure assessment, we developed a method to estimate residence times for a suite of SVOCs based on both the mass distribution of the compound between the “mobile phase” (air and particles in the carpet) and the “non-mobile phase” (the carpet fibers and pad) and the removal rates resulting from air exchange and surface cleaning (Shin et al., 2013a). We compared model results to changes in chlorpyrifos air concentrations collected at two time points, approximately one year apart, during the time period chlorpyrifos was banned for indoor use. The large fraction of SVOCs in the non-mobile phase from this study supports the premise that SVOCs are persistent in the indoor environment.

As a more reliable exposure-based chemical prioritization approach is needed to evaluate and prioritize more than tens of thousands of chemicals in a rapid and efficient manner, we estimated intake fractions for a suite of indoor organic compounds (Shin et al., 2012). We used the intake fraction as an output metric because it is a useful concept for expressing source-to-intake relationships. We calculated intake through various exposure pathways based on human activity patterns, chemical release scenarios, and the mass distribution from a fugacity-based indoor model.

In the second year, we (1) evaluated environmental modeling and sampling data with biomarker data to identify sources and routes of exposure and (2) determined source strength of SVOCs indoors based on dust levels. In the evaluation study, we compared the magnitude and variation of modeled polycyclic aromatic hydrocarbons (PAHs) exposures resulting from emissions to outdoor and indoor air and estimated exposure inferred from biomarker levels (Shin et al., 2013b). The comparison of PAH biomarkers with exposure variability estimated from models and sample data for various exposure pathways supports that both indoor and outdoor models are needed to capture the sources and routes of exposure to environmental contaminants. For most chemicals there is limited information available about how the use in consumer products and building materials result in releases to indoor environments and then to human exposures. Therefore, we used a fugacity-based indoor mass-balance model to estimate emission rates of SVOCs that account for the measured dust concentrations collected in 30 U.S. homes (Shin et al., 2014a). The combined dust-assay modeling approach shows promise for estimating indoor emission rates for SVOCs.

In the third year, we first conducted a simulation study to help interpret source contributions to human body burden using the correlation coefficients between environmental measurements and biomarkers. This simulation study addresses current knowledge gaps regarding causes for correlations between environmental and biomarker measurements and explores the underappreciated role of variability in...
disaggregating exposure attributes that contribute to biomarker levels (Shin et al., 2014b). Second, information about the distribution of chemical-production mass with respect to various use and thus resulting releases to various environmental media is a major and unavailable input for calculating population-scale exposure estimates. Thus, we allocated chemical production volumes to the various modes of entry using intake fractions and national biomonitoring data. The approach of the source apportionment study provides insights on confronting data gaps to improve population-scale exposure estimates used for high-throughput chemical prioritization (Shin et al., 2014c).

As part of the final phase of this project, focused on the prioritization of chemicals based on exposure estimates and in vitro bioactivity data, we worked together with two other expert research groups (University of Michigan at Ann Arbor in collaboration with the Technical University of Denmark, and the University of Toronto at Scarborough). We first compared the results of exposure estimates between groups and then compared the conservative exposure estimates with in vitro bioactivity values (Shin et al., 2014d).

**Implications:** Tox21 (ToxCast™ and the National Toxicology Program) supports the development of exposure screening tools to complement current hazard screening tools for prioritization and risk assessment. This project couples and extends existing exposure models, which will provide great utility and also great credibility to these models, potentially increasing their use and acceptance in certain applications, including risk-based decision making. It also extends screening tools, which are currently based on hazard alone, to include exposures. Additionally, this project will engage the U.S. Environmental Protection Agency to develop stakeholder agreement around appropriate screening tools and will mobilize ground-truthing of exposure screening tools.

**Key words:** exposure, residence times, intake fractions, exposure modeling, exposure-based chemical screening tools, source strength, production volumes

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**Peer-reviewed publication(s):**


This abstract was prepared by the principal investigator for the project. Please see [www.americanchemistry.com/lri](http://www.americanchemistry.com/lri) for more information about the LRI.
Other publication(s):


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