The landscape of existing models for high-throughput exposure assessment

Jolliet, O.; Fantke, Peter; Huang, L.

Published in:
Abstract book - ISES 27th Annual Meeting

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

2017 Annual Meeting

ISES2017 ABSTRACT BOOK

Integrating Exposure Science Across Diverse Communities

Research Triangle Park, NC, USA

October 15-19, 2017

INTERNATIONAL SOCIETY OF EXPOSURE SCIENCE

Abstract: FDA's Total Diet Study (TDS), initiated in 1961, continuously monitors concentrations of lead and other contaminants in about 280 foods, based on quarterly sampling and analysis of these foods in four regions of the U.S.. Over the past three years, FDA has focused attention on modernizing and revitalizing the TDS program by developing a data management system for trend analysis; updating analytical methods to improve data quality; improving the sample collection protocol; and updating the TDS website. TDS concentration data for lead and other contaminants include high proportions of values below the limit of detection (LOD), and this presents challenges for statistical calculations. FDA has developed a novel statistical method, clustered zero-inflated lognormal distribution analysis, to estimate central tendency concentrations and confidence intervals in food-analyte pairs.

Keywords: C-food, B-metals, A - exposure measurement

MO-SY-F3: Quantitative High-Throughput Exposure Methods for Chemical Alternatives and Comparative Risk Assessment

MO-SY-F3-148

The landscape of existing models for high-throughput exposure assessment

O. Jolliet[1], P. Fantke[2], L. Huang[1]; [1]University of Michigan, Ann Arbor, MI, [2]Technical University Denmark, Lyngby, Denmark

Abstract: Models are becoming increasingly available to model near-field fate and exposure, but not all are suited for high throughput. This presentation evaluates the available models for modeling exposure to chemicals in cosmetics, cleaning products, food contact and building materials. It assesses their applicability to quantitative high throughput exposure assessment in CAA and CRA, looking in particular at the following characteristics: validity of main assumptions; availability of analytical solutions and model parsimony; availability of methods to estimate key inputs for a large number of chemicals and ability to easily handle large datasets. For building materials a series of diffusion-based models have been developed to predict the chemicals emissions from building materials to indoor air, but existing models require complex analytical or numerical solutions, which are not suitable for LCA or HTS applications. Thus, existing model solutions needed to be simplified for application in LCA and HTS, and a parsimonious model has been developed by Huang et al. (2017) to address this need. For SVOCs, simplified solutions do exist, assuming constant SVOC concentrations in building materials and steady-state in indoor air (Little et al., 2012; Liu et al., 2013), but they do not well account for SVOC sorption into indoor surfaces and absorption into human skins (Huang et al., 2017). Thus a more comprehensive simplified solution is needed for SVOCs . For personal Care Products, a mass balance model that accounts for skin permeation and volatilization as competing processes and that requires a limited number of readily available physiochemical properties would be suitable for LCA and HTS purposes. Thus, the multi-pathway exposure model for chemicals in cosmetics developed by Ernstoff et al.constitutes a suitable basis and can be refined in the future. The review will also address models available for modeling chemicals in cleaning products and other indoor used chemicals.

Keywords: A-chemical prioritization, A-exposure models, A - population exposure, A-indoor environment, B-SVOCs

MO-SY-F3-149

Identifying Potential Alternatives using Chemical Functional Use

K. Phillips[1], J. Wambaugh[2], C. Grulke[2], K. Dionosio[1], K. Isaacs[1]; [1]U.S. Environmental Protection Agency, Research Triangle Park, NC, [2]U.S. Environmental Protection Agency, Research Triangle Park, NC

Abstract: The National Research Council noted in its 2014 report *A Framework to Guide Selection of Green Alternatives* that "focusing on function can provide opportunities for innovation in safer chemicals