Migration modeling to estimate exposure to chemicals in food packaging for application in highthroughput risk-based screening and Life Cycle Assessment

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

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

exposure to chemicals and expand the knowledge base for further development of chemical exposure pathways and models.

Keywords: A-exposure models, A-indoor environment, A-sampling methods, B-SVOCs

MO-PL-E2: Food Packaging

MO-PL-E2-115

A Quantitative Property-Property Relationship for Estimating Packaging-Food Partition Coefficients of Organic Compounds

L. Huang[1], A. Ernstoff[2], H. Xu[1], S. Lu[1], P. Fantke[3], O. Jolliet[1]; [1]University of Michigan, Ann Arbor, MI, [2]Quantis Lausanne, Lausanne, Switzerland, [3]Technical University of Denmark, Lyngby, Denmark

Abstract: Organic chemicals encapsulated in beverage and food packaging can migrate to the food and lead to human exposures via ingestion. The packaging-food (K_{pf}) partition coefficient is a key parameter to estimate the chemical migration from packaging materials. Previous studies have simply set K_{pf} to 1 or 1000, or provided separate linear correlations for several discrete values of ethanol equivalencies of food simulants (EtOH-eq). The aim of the present study is to develop a single quantitative property-property relationship (QPPR) valid for different chemical-packaging combinations and for water or different EtOH-eq values. We compiled datasets of measured K_{pf} from 3 studies, which contained 302 data points of 152 chemicals in LDPE and HDPE (low and high density polyethylene) at 25 °C for EtOH-eq values ranging from 0% (water) to 95%. A multiple linear regression (MLR) model was developed to predict K_{pf} as a function of the chemical's K_{ow}, the EtOH-eq, the packaging type and an interaction term between K_{ow} and EtOH-eq. The model shows good fitting performance of the experimental datasets with adjusted R-square of 0.92. All predictors are highly significant except the packaging type, probably because only two packaging types are included. This preliminary QPPR demonstrates that the K_{pf} for various chemical-packaging-food combinations can be estimated by a single linear correlation. Based on more than 1000 collected K_{pf} in 15 materials, we will present extensive results for other packaging types and different temperatures. This QPPR provides a comprehensive correlation method to estimate the K_{pf} for a wide range of chemical-packaging-food combinations, and thus facilitate high-throughput estimates of human exposures to chemicals encapsulated in food contact materials.

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

MO-PL-E2-116

Migration modeling to estimate exposure to chemicals in food packaging for application in high-throughput risk-based screening and Life Cycle Assessment

A. S. Ernstoff[1], O. Jolliet[2], L. Huang[2], P. Fantke[1]; [1]DTU, Kgs. Lyngby, Denmark, [2]University of Michigan, Ann Arbor, MI

Abstract: Specialty software and simplified models are often used to estimate "worst-case" migration of potentially toxic chemicals from packaging into food. Current approaches, however, cannot efficiently and accurately provide estimates of migration for emerging applications, e.g. in Life Cycle Assessment and risk prioritization and screening. To fulfill the need for a migration model flexibly suitable for such tools, we develop an accurate and rapid (high-throughput) approach. The developed model estimates the fraction of an organic chemical migrating from polymeric packaging into food for user-defined scenarios and requires limited parameters (i.e. physicochemical properties). Several hundred step-wise simulations optimized the coefficients of the model to cover a wide-range of scenarios (e.g. packaging thickness, food etc.). The developed model, implemented in a disseminatable spreadsheet, nearly instantaneously estimates migration from packaging into food for user-defined scenarios, and has improved performance over common model simplifications. The common practice of setting the package-food partition coefficient = 1 for specific "worst-case" scenarios is insufficient to predict the equilibrium concentration in food for

diverse scenarios. Therefore a partition coefficient model, as a function of a chemical's octanol-water partition coefficient and a food's ethanol-equivalency, was also developed. When using measured diffusion coefficients the model accurately predicted (R^2 = 0.9, SE = 0.5) hundreds of empirical datapoints for various scenarios. Diffusion coefficient modeling, which determines the speed of chemical transfer from package to food, was found as a major contributor to uncertainty and decreased model performance (R^2 = 0.5, SE = 1). In all, this study provides a migration modeling approach that rapidly estimates the fraction migrated for emerging screening and prioritization approaches. To estimate exposure, chemical concentrations in packaging are essential.

Keywords: A-exposure models, C-food, A-life cycle analysis, A-chemical prioritization, C-consumer products

MO-PL-E2-117

Consumer Exposures to Engineered Nanomaterials through Dietary Sources

K. Grieger; RTI International, Research Triangle Park, NC

Abstract: Engineered nanomaterials (ENMs) are currently used in a wide range of consumer products, including food, dietary supplements, and food packaging. In addition, ENMs are also being developed for advanced water treatment technologies to help secure safe, sustainable water supplies. The use of ENMs in consumer products such as food and drinking water applications has been attractive to material scientists, engineers, and product developers given that ENMs often display unique, novel properties compared to their bulk counterparts. At the same time, there have also been safety concerns and questions raised regarding the use of ENMs in consumer products and other applications. The overall extent to which consumers are exposed to ENMs through dietary sources such as food and drinking water is still largely unknown at this time. This is largely due to the lack of robust analytical techniques for detection, characterization, and quantification of ENMs in food and drinking water matrices, as well as other challenges related to assessing consumer and environmental exposures to ENMs. This presentation provides an overview of consumer exposures to ENMs through dietary sources along with some concerns regarding these exposures. Recommendations are also made to stakeholder groups for the sustainable development and use of ENMs in food and drinking water treatment applications.

Keywords: A-nanotechnology, B-nanoparticles, C-consumer products, C-food

MO-SY-F2: Pathways and mechanisms linking exposure to the natural environment with health and well-being benefits - Part 2

MO-SY-F2-118

Using Health Effect Biomarkers to Characterize Benefits of Urban Green Spaces

A. I. Egorov, S. Griffin, R. Converse, J. Styles, E. Sams, A. Wilson, R. Baldauf, V. Isakov, L. E. Jackson, T. Wade; United States Environmental Protection Agency, RTP, NC

Abstract: Greater availability of urban green spaces has been linked to improved mental and physical health, and reduced mortality. Relative contributions of hypothesized pathways to improved health, such as relaxation and stress alleviation; enhanced physical activity; reduced exposure to air pollution, noise and heat; and beneficial exposure to natural allergens and microbes, remain to be characterized. The objective of an ongoing research project at U.S. EPA is to characterize subtle biological changes associated with long-term exposure to green space using a panel of biomarkers of metabolic, neuroendocrine and immune function, and to produce novel information on pathways to health. A pilot cross-sectional study in the Durham-Chapel Hill, NC area used 1-meter resolution data on trees and herbaceous vegetation within 500 m of residences derived from the U.S. EPA EnviroAtlas land cover