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ABSTRACT BOOK

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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

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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

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

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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