Progress in High Throughput Exposure Assessment for Prioritizing Human Exposure to Environmental Chemicals

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For thousands of chemicals in commerce, there is little or no information about exposure or health and ecological effects. The US Environmental Protection Agency (USEPA) has ongoing research programs to develop and evaluate models that use the often minimal chemical information available for rapidly assessing the potential for exposure. Two exposure models that passed an evaluation of their ability to make quantitative predictions of exposure based on limited information (Mitchell et al, 2013), were evaluated for their ability to predict biomonitoring data from the National Health and Nutrition Examination Survey (NHANES) for about 100 chemicals found in urine samples. The two models were found to have essentially no skill in predicting exposures inferred from the biomonitoring data, but a binary indicator of whether the exposure was likely to be near-field (i.e., from indoor emissions or products likely to be directly encountered) explained a significant fraction of the total variance in inferred exposure (Wambaugh et al, 2013). Further analysis has refined the nature of the 'near-field' predictor, and was able to explain about half the variance in the exposures inferred from NHANES biomonitoring data using a regression-like model on indicators for use categories and an estimate of production volume (Wambaugh et al, 2014). This heuristic model can make exposure predictions for almost 8000 chemicals of interest, but, since the predictions are based on regression modeling of a small number of chemicals, the predictions are subject to question based on domain of applicability concerns. SHEDS-HT (Isaacs, et al., 2014) is a probabilistic exposure model for chemicals with near-field and dietary exposure. While it can currently make predictions for only 39 chemicals of the NHANES evaluation dataset, it can explain about 40% of the variance of inferred exposure for those chemicals. This compares favorably with the empirical model, since no calibration against the evaluation data was involved in the SHEDS-HT fits. A critical feature of this model evaluation and development is the incorporation of data-derived prediction uncertainties. This allows an objective answer to the question of whether a given model is "fit for purpose", by referring directly to a prespecified level of error. This abstract does not necessarily reflect U.S. EPA policy.