Development of Physiologically Based Pharmacokinetic (PBPK) Models within Bayesian Framework and Roles of Artificial Intelligence Technologies in Human Health Risk Assessment: A Case Study with Perfluorooctane Sulfonate (PFOS)

Wei-Chun Chou, PhD
Research Assistant Professor
Department of Environmental and Global Health
Center for Environmental and Human Toxicology
University of Florida, USA

Abstract

Inter- and intra-species variability in chemical pharmacokinetics and toxicological endpoints results in a significant difference in the estimation of reference dose (RfD), thus leading to an enormous challenge in human health risk assessments. Recently, we developed an integrated framework by combing Bayesian statics with physiologically based pharmacokinetic (PBPK) models to characterize uncertainty and variability between species, individuals, and life stages. This Bayesian population PBPK model has been used in the estimation of RfD from interspecies extrapolations, simulation of the internal dose metrics for potentially sensitive subpopulations, and prediction of in vitro to in vivo extrapolation (IVIVE) of kinetic and toxicity data. In this presentation, I will introduce how we develop mechanistic PBPK model structure in different species, chemicals, and life stages within the Bayesian hierarchical framework and application for the per-and poly-fluoroalkyl substances (PFAS) risk assessments. In addition, based on my perspective, I will share a new paradigm to explain how the integration of the PBPK model and artificial intelligence (AI) and utilization in the areas of toxicology and risk assessment.