Optimization of the cumulative risk assessment of pesticides and biocides using computational techniques: Pilot project - DTU Orbit (28/09/2019)

This pilot project is intended as the first step in developing a computational strategy to assist in refining methods for higher tier cumulative and aggregate risk assessment of exposure to mixture of pesticides and biocides. For this purpose, physiologically based toxicokinetic (PBTK) models were developed for two compounds, tebuconazole and prochloraz, and a binary mixture of these compounds in two species, rat and human. PBTK models can be used to estimate the concentration levels (internal doses) of toxic substances and their metabolites in blood and tissue, by a collection of differential equations, and parameters describing species physiology and ADME (absorption, distribution, metabolism and elimination) characteristics of the chemicals. Sufficient data were found to determine the parameters needed for the PBTK model development. The PBTK models were validated on plasma and tissue concentration level data of tebuconazole in rabbit, and in most cases the predictions were seen to be within a factor of two compared to the experimental data. Also simple blood concentration measurements for both compounds from a mixture study in rat, and other data were used to validate and evaluate the models. Exposure scenarios were constructed based on findings of pesticide residues in food of ordinary consumers, and assessment of dermal exposure of professional workers. PBTK simulations were carried using these scenarios.

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