BIO-FI: LEVERAGING THE POWER OF BIOLOGICAL BIG DATA FOR ADVANCED ANALYTICS AND MODELING OF CHEMICAL AND BIOLOGICAL THREATS

Leveraging Regulatory Models And Data For Cb Operational Hazard Prediction

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SRC, Inc. is working with ARA and DTRA Reachback to enhance current operational models in HPAC and extend current hazard prediction capability to process emerging threat chemicals, develop combined effect output for chemical mixtures, augment percutaneous exposure calculations, and integrate read-across strategies. To facilitate these development efforts SRC is leveraging data and models developed on parallel efforts for DTRA, CDC, and EPA.

Current efforts are underway with DTRA Reachback to augment the Combined Logical Estimation Application for Rapid Results (CLEARR) software tool for use with HPAC as an input generator for chemicals that may not be included in the current vetted and approved material files. SRC is building an automated material file module (PropCast) aimed at creation of an HPAC xml-based material file using only a chemical structure. This will allow HPAC users to generate a screening level hazard prediction output on the fly using a combination of experimental, estimated, and extrapolated values produced from CLEARR.
In parallel, SRC is working with ARA to develop a method to augment the hazard prediction of chemical mixtures as calculated in FXCODA. To accomplish this, SRC is exploring the use of methods developed by risk assessors and regulators at the CDC's ATSDR branch to determine the health impacts of multi-component mixtures. Specifically, the hazard index (HI) approach is a methodology used by several federal agencies for screening level assessments. The methodology assesses hazards from mixtures based upon the assumption that dose additivity is valid. Exposures or doses for components of the mixture are compared with an exposure level deemed acceptable or safe.

SRC is also leveraging percutaneous exposure models developed by the EPA and implemented in CLEARR to augment FXCODA. Computing the effective dose of an exposed group of individuals is a combination of three different exposures: the inhaled dose, the percutaneous vapor dosage, and the percutaneous liquid dosage per current methodology. CLEARR has incorporated Quantitative Structure Activity Relationships (QSARs) to estimate dermal permeability coefficients (Kp) which are required to estimate the dermal absorbed dose for percutaneous liquid and vapor exposures for FXCODA and ultimately HPAC. Lastly, SRC is working to leverage read-across strategies based on chemical similarity, toxidrome, or mode of action analysis which can be used to capture toxicological lethality values of emerging threats or substances lacking experimental data required in HPAC material files and used by FXCODA to estimate casualties.

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